IUCLID

Data Set

Existing Chemical	:	ID: 583-78-8
CAS No.	:	583-78-8
Generic name	:	Phenol, 2,5-dichloro
Producer related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Substance related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	13.12.2007
Revision date	:	
Date of last update	:	13.12.2007
Number of pages	:	27
Chapter (profile)	:	Chapter: 1.0.1, 1.2, 1.6.1, 1.6.2, 1.8.1, 1.8.3, 1.8.4, 1.8.5, 1.10, 1.11, 2, 3, 4, 5, 7
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.2 SYNONYMS AND TRADENAMES

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

2.1 MELTING POINT

Value	:	59 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	EPIWIN v3.20 MPBPWIN v1.42 Output: ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 233.74 deg C (Adapted Stein and Brown Method) Melting Point: 94.72 deg C (Adapted Joback Method) Melting Point: 22.82 deg C (Gold and Ogle Method) Mean Melt Pt : 58.77 deg C (Joback; Gold,Ogle Methods) Selected MP: 46.79 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions Handbook data
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1) (2)

2.2 BOILING POINT

Value	:	211 °C at
Decomposition	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	EPIWIN v3.20, MPBPWIN v1.42 Output: ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 233.74 deg C (Adapted Stein and Brown Method)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions Handbook data
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1) (2)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .08 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Remark	:	EPIWIN v3.20, MPBPWIN v1.42 Output: ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 233.74 deg C (Adapted Stein and Brown Method) Melting Point: 94.72 deg C (Adapted Joback Method) Melting Point: 22.82 deg C (Gold and Ogle Method) Mean Melt Pt : 58.77 deg C (Joback; Gold,Ogle Methods) Selected MP: 46.79 deg C (Weighted Value) Vapor Pressure Estimations (25 deg C): (Using BP: 211.00 deg C (exp database)) (Using MP: 59.00 deg C (exp database)) VP: 0.0541 mm Hg (Antoine Method) VP: 0.0458 mm Hg (Modified Grain Method) VP: 0.146 mm Hg (Mackay Method) Selected VP: 0.0458 mm Hg (0.060914 hPa) (Modified Grain Method)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Reliability	:	(2) valid with restrictions Literature value
Flag	:	Critical study for SIDS endpoint

13.12.2007 (3) (1)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 3.06 at 25 °C
pH value	:	
Remark	:	Supported by EPIWIN calculated value value of 2.80
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions Literature value
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	= 2000 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	other: slightly soluble

Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	

Remark : Remarks:
1. Secondary literature. No source or method of determination is given.

There is an experimental database match given in WSKOW v1.41 in EPIWIN 3.20:

Experimental Water Solubility Database Match:
Name : 2,5-DICHLOROPHENOL
CAS Num : 000583-78-8
Exp WSol : 2000 mg/L (25 deg C)
Exp Ref : CHEM INSPECT TEST INST (1992)

EPIWIN v3.20, WSKOW v.41 Output:

---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 2.80
Log Kow (experimental): 3.06
Cas No: 000583-78-8
Name : 2,5-Dichlorophenol
Refer : Hansch,C et al. (1995)
Log Kow used by Water solubility estimates: 3.06

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
Phenol	0.580

Log Water Solubility (in moles/L) : -2.424
Water Solubility at 25 deg C (mg/L): 614.2

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(4) not assignable secondary literature (remark 1)
Flag	:	Critical study for SIDS endpoint

26.12.2001 (5) (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	ca. .0000000000069851 cm³/(molecule*sec)
Degradation	:	= 50 % after 18 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using AOPWIN v1.92 in EPIWIN 3.20.
Result	:	AOP Program (v1.92) Results: ========== SMILES : c1(c(ccc(c1)CL)CL)O CHEM : MOL FOR: C6 H4 CL2 O1 MOL WT : 163.00 --------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 6.8451 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 6.9851 E-12 cm3/molecule-sec HALF-LIFE = 1.531 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 18.375 Hrs -------- SUMMARY (AOP v1.91): OZONE REACTION ---------- ****** NO OZONE REACTION ESTIMATION ****** (ONLY Olefins and Acetylenes are Estimated)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	
Test substance	:	

Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (6)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	

Method : Fugacity was determined using the EQC Level III model as found in EPIWIN 3.20. Equal emissions to air, water and soil were assumed. Parameters used were the default values found in EPIWIN.

Result : Level III Fugacity Model (Full-Output):

==========

Chem Name : Phenol, 2,5-dichloro-
Molecular Wt: 163
Henry's LC : 4.77e-007 atm-m3/mole (Henrywin program)
Vapor Press : 0.0458 mm Hg (Mpbpwin program)
Liquid VP : 0.0752 mm Hg (super-cooled)
Melting Pt : 46.8 deg C (Mpbpwin program)
Log Kow : 3.06 (Kowwin program)
Soil Koc : 471 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.842	36.7	1000
Water	17.8	900	1000
Soil	80.9	1.8e+3	1000
Sediment	0.463	8.1e+3	0

	Fugacity	Reaction	Advection	Reaction	Advection

	(atm)	(kg/hr)	(kg/hr)	(percent)	(percent)
Air	4.35e-11	548	291	8.3	9.68
Water	8.96e-12	472	613	15.7	20.4
Soil	3.91e-11	1.07e+3	0	35.8	0
Sediment	9.5e-12	1.37	0.319	0.0455	0.0106

Persistence Time: 1.15e+003 hr
Reaction Time: 1.65e+003 hr
Advection Time: 3.82e+003 hr
Percent Reacted: 69.9
Percent Advected: 30.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 36.74
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.482 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : 2,5-dichlorophenol, CAS 583-78-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
18.10.2007 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Contact time : 4 day(s)
Degradation : = 52 (±) % after 4 day(s)
Result :
Deg. product :
Method :
Year : 1966
GLP : no data
Test substance :

Remark : The material is reported to undergo 54% ring degradation in 4 days with acclimated sludge. It cannot be determined if this test substance is considered readily biodegradable by OECD criteria.
Result : The biological degradation of chlorophenols in activated sludge was studied. 2,5-Dichlorophenol was more resistent to degradation than 2,4-dichlorophenol. While 2,4-dichlorophenol was 100% degraded, including ring degradation, in five days, 2,5-dichlorophenol was only 52% ring-degraded in four days.

[USEPA; Ambient Water Quality Criteria Doc: Chlorinated Phenols p.C-29 (1980) EPA 440/5-80-032]**PEER REVIEWED** As cited in HSDB update of 8-09-2001

Source : Toxicology and Regulatory Affairs Flemington NJ
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
18.10.2007 (7)

Type : aerobic
Inoculum : activated sludge
Concentration : 100 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : (±) % after
Result : under test conditions no biodegradation observed
Deg. product :
Method : OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year :
GLP :
Test substance :

Method : Conducted according to MITI-I (equivalent to OECD TG 301-C). Analyses by BOD, TOC and HPLC.
Result : Results: by BOD - 5% degradation; by TOC, 8% degradation; by HPLC, 3% degradation.
Reliability : (2) valid with restrictions
18.10.2007 (8)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	other: Platichthys flesus (Starry European flounder)
Exposure period	:	96 hour(s)
Unit	:	µg/l
LC50	:	= 3290 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	
Year	:	1994
GLP	:	
Test substance	:	

Method	:	The test was conducted in seawater. The test material was prepared in sodium hydroxide as a solvent.
Test condition	:	Test temperature was 6 degrees C, pH was 8, and salinity was 5 ppt.
Test substance	:	2,5-Dichlorophenol, 98-99% purity
Reliability	:	(4) not assignable Insufficient detail provided.

13.12.2007 (9)

Type	:	static
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	µg/l
LC50	:	= 3300 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	
Year	:	1988
GLP	:	
Test substance	:	

Result	:	The EC50 was 3300 ug/L (confidence interval 2500 - 4500 ug/L).
Reliability	:	(4) not assignable Insufficient detail provided.

18.10.2007 (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2475 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	female
Number of animals	:	10
Vehicle	:	other: sesame oil
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source:no data - Age: no data - Number:10/dose - Weight at study initiation: 80-97 g - Controls: no ADMINISTRATION: - Doses: 1600, 2500, 4000 mg/kg bw - Doses per time period: single (gavage) - Volume administered not indicated - Post dose observation period: 14 days - food withheld 16 hr before to 2 hr after dosing EXAMINATIONS: Necropsy of all animals with macroscopic examination. Body weight (pre-dosing, days 7 and 14) STATISTICAL METHOD: probit (Linder and Weber)
Result	:	MORTALITY: - Number of deaths at each dose: 1600, 2500 and 4000 mg/kg bw 1/10, 4/10 and 10/10 - Time of death: deaths within 24 hours after dosing CLINICAL SIGNS: in dying animals: excessive breathing, equilibrium disturbance and tremor, moreover tonic clonic spasms in the ventral region. In the highest dose, these signs occurred immediately after dosing. NECROPSY FINDINGS: No abnormal findings were noted in surviving animals. In decendents: clear dilated bloodvessels on the intestines BODY WEIGHT: normal body weight gain in surviving animals No data on decendents POTENTIAL TARGET ORGANS: intestines
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-Dichlorphenol), purity not indicated,

cristalline form

Conclusion	:	LD50 2475 mg/kg bw (95% CI 2101-2916 mg/kg bw)
Reliability	:	(2) valid with restrictions 1. The information was essentially confined to what is included in the current summary 2. only females were tested 3. no individual data were present

13.12.2007 (11)

Type	:	LD50
Value	:	946 - 1600 ml/kg bw
Species	:	mouse
Strain	:	other: CD-1 ICR
Sex	:	male/female
Number of animals	:	100
Vehicle	:	other: corn oil
Doses	:	
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Age: adult - Number: 10 males, 10 females per dosage level - Weight at study initiation: - Controls: no data ADMINISTRATION: - by gavage - Doses: 5 levels, levels not indicated - Volume administered or concentration: 10 mL/kg body weight - food withheld for 2 h after dosing - Post dose observation period: 14 days EXAMINATIONS: behavior and visible health, time of death, necropsy of animals that died during the test STATISTICAL METHOD: Log probit analysisof Finney; Litchfield, Wilcoxon.
Remark	:	Remarks: 1. Remarks: The article contains a summary rather than a full report. Information is essentially confined to what is mentioned in this summary. Especially no detailed results are given.
Result	:	LD50 male: 1600 mg/kg bw (confidence limits: 1233-2075 mg/kg bw); LD50 female: 946 mg/kg bw (confidence limits: 623-1438 mg/kg bw)
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity 98%
Reliability	:	(4) not assignable secondary literature (remark 1)
Flag	:	Critical study for SIDS endpoint

13.12.2007 (12)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 185000 mg/m³

Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10
Vehicle	:	
Doses	:	
Exposure time	:	4 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: no data
- Age: no data
- Weight at study initiation: 216-243 g
- Number of animals: 10 (5 male, 5 female)

ADMINISTRATION:
- Type of exposure: inhalation (whole body)
- Exposure duration: 4 hours
- Concentrations: 50000 mg/m3; 185000 mg/m3
- Particle size: no data
- Type or preparation of particles: no data
- Air changes: no data

EXAMINATIONS: clinical signs during and immediately following exposure; macroscopy

Result :

MORTALITY:
- Number of deaths at each dose:50000 mg/m3: none; 185000 mg/m3: 2 (females)
- Time of death: during exposure (both)

CLINICAL SIGNS: 50000 mg/m3, (all rats): increased/decreased motor activity, eye squint, erythema, lacrimation, salivation, clear nasal discharge, ocular and nasal porphyrin discharge, slight dispnoea. The symptoms disappeared in all rats 24 hours after exposure
185000 mg/m3, (all rats): The same symptoms as at 50000 mg/m3, with addition of marked dispnoea, corneal opacity, ataxia, sedation and body jerking. The symptoms disappeared 72 hours after exposure (one rat exhibiting nasal porphyrin discharge at day 10)

NECROPSY FINDINGS: congested lungs and liver, slight corneal opacity (in the animals that died)

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions 1. The information included in the report was confined to what is included in the current summary 2. No information on body weight was presented

13.12.2007 (13)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 8000 mg/kg bw
Species	:	rabbit

Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	
Doses	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: no data - Age: no data - Weight at study initiation: 2387-2970 g - Controls: no data ADMINISTRATION: - Area covered: no data - Occlusion: yes - Vehicle: not applicable (applied as powder) - Doses: 1000, 2000, 4000 and 8000 mg/kg bw - Removal of test substance: washed with tepid tap water EXAMINATIONS: observations for mortality during 14 days; body weight at start and day 14 STATISTICAL METHOD: Thompson, W.R., Bact. Rev.: 115-145, 1947
Result	:	MORTALITY: - Number of deaths at each dose: none CLINICAL SIGNS: no data BODY WEIGHT: decreased body weight in both females at 2000 mg/kg bw , in one male and one female at 4000 mg/kg bw and in males at 8000 mg/kg
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions 1. The information included in the report was confined to what is included in the current summary 2. Only 4 animals per group (animals not of one sex only), of which one underwent skin abrasion (OECD 402: at least five animals per dosage group, no abrading of the skin) 3. The size of the application area was not indicated

13.12.2007 (14)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	4 weeks
Frequency of treatm.	:	5 days/week, 6 hours/day
Post exposure period	:	
Doses	:	0.1, 0.3 and 1.0 mg/L
Control group	:	yes, concurrent no treatment
LOAEL	:	= .1 - mg/l
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Age: 8 weeks
- Weight at study initiation: males 206-230 g,females 192-224 g
- Number of animals: 10/sex/treatment

ADMINISTRATION / EXPOSURE
- Exposure period: 4 weeks, 6 hours/day, 5 days/week
- Route of administration: inhalation (whole body)
- Doses: 0.1, 0.3 and 1.0 mg/L
- Particle size: not applicable (vapour)
- Air changes: 2-16/hour

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: twice daily
- Body weight: pre-treatment and weekly thereafter
- Haematology: after 4 weeks: haematocrit, Hb, erythrocyte count, (differential) leucocyte count, MCV, MCH(C).
- Biochemistry: after 4 weeks: glucose, BUN, ALP, ALAT, ASAT
- Urinalysis: after 4 weeks accoridng to OECD 407

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: liver, spleen, kidneys, heart, lungs, brain, adrenals, thyroid, pituitary
- Macroscopic: all tissues (see microscopy) from all animals
- Microscopic: from controls and high dose group: nasal turbinates, trachea, lung, spleen, pancreas, stomach, duodenum, uterus, prostate, kidneys, urinary bladder, ovaries, testes, bone marrow, heart, mediastinal and mesenteric lymphnodes, colon, liver, adrenals, olfactory bulb, thyroid, parathyroid, brain , eye, pituitary, gross lesions
from other dose groups: nasal turbinates, trachea, lung, liver

ANALYSES:
- Method: nominal concentrations by weighing of the vaporisation flask before and after exposure

Result	:	STATISTICAL METHODS: ANOVA, Bartlett's test, Dunnett's test ANALYSES: - Nominal concentration: at 0.1, 0.3 and 1.0 mg/L 0.07-0.28, 0.07-1.09 and 0.45-1.36 mg/L respectively. TOXIC RESPONSE/EFFECTS BY DOSE LEVEL: - Mortality: none - Clinical signs: Nasal irritation with or without discharge in all treatment groups and controls Ocular irritation and discharge in all treatment groups Salivation in 8 males and 4 females at 0.3 mg/L and in 7 males and 7 females at 1.0 mg/L Dyspnoea in one male and 7 females at 0.3 mg/L Incidental findings respiratory distress, skin irritation, cloudy spots on eyes, decreased activity and soaked abdomen - Body weight gain: decreased at 0.3 mg/L during week 2-4 and at 1.0 during week 1-4. - Haematology: Hb increased at the high dose group, No. of leucocytes increased in females at 0.3 and 1.0 mg/L - Clinical chemistry: ASAT increased in high dose males and females - Urinalysis: no treatment related effects - Organ weights: Decreased absolute liver and brain weight in males at 0.3 and 1.0 mg/L Increased relative lung weight in females at 1.0 mg/L Decreased absolute heart weight in males at 0.3 mg/L Increased relative kidney weight in all treated males - Gross pathology: Brown cyanotic/discolored areas, foci and atelectasis in the lungs were seen in 1-2 animals/sex/treatment and in controls. At 1.0 mg/L the incidence was slightly increased in females. Other incidental effects included haemorrhagic/hyperemic lymphnodes, effects on stomach mucosa, pale/discolored liver areas/foci and haemorrhagic foci and discoloration of the kidneys. - Histopathology: Inflammatory cell and lymphocyte infiltrate, macrophage aggregation and septal fibrosis in the lungs of all treated animals Inflammation of the nasal cavity (mucosa) in animals at 1.0 mg/L Lymphocytic infiltrate, inflammation, foci and necrosis of the liver in treated and control animals. The incidence in control animals was slightly lower (9/20) compared to treatd animals (14-16/20). STATISTICAL RESULTS: The effects on body weight, organ weight and bloodparameters were statistically significant. None of the effects showed a clear concentration-response relationship.
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Conclusion	:	LOAEL 0.1 mg/L based on liver effects. Other effects seen were related to a weight decrease (organ weights) or could be attributed to irritant properties of the test substance (effects in the respiratory tract).

Reliability	:	(2) valid with restrictions 1 No analyses for actual concentration, homogeneity and stability were performed. 2 The effects on organ weights are expected to be related to the decreased body weight. 3 No blood clotting parameters were detemined

13.12.2007 (15)

Type	:	
Species	:	rabbit
Sex	:	male/female
Strain	:	New Zealand white
Route of admin.	:	dermal
Exposure period	:	21 days
Frequency of treatm.	:	5 days/week, 6 hours/day
Post exposure period	:	
Doses	:	1.0, 10 and 100 mg/kg bw
Control group	:	other: distilled water
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Weight at study initiation: 2171-2921 g (males), 2028-3146 g (females)
- Number of animals: 4/sex/treatment
- Source: HARE Rabbits Research, Hewitt, NJ

ADMINISTRATION / EXPOSURE
- Exposure period: 21 days, 5 days/week, 6 hours/day
- Route of administration: dermal
- Doses: 1.0, 10.0 and 100 mg/kg bw; water control
- Vehicle: not applicable (substance was melted at 60 C before application)
- Total volume applied: =<0.1 mL/kg
- Area treated: 10% of body surface (at 1.0 and 10 mg/kg bw every day another area was treated)
- Occlusion: no (a collar was applied to prevent oral ingestion of the test substance)
- Removal of test substance: washed with tepid water after 6 hours

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: daily
- Dermal effects: before and after exposure
- Body weight: weekly
- Haematology/biochemistry: pre-test and after 21 days:
haematocrit, Hb, erythrocyte count, (differential) leucocyte count, MCV, MCH(C)
glucose, BUN, ALP, ALAT, ASAT
- Urinalysis: pre-test and after 21 days according to OECD 410

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: liver, spleen, kidneys, brain, adrenals, thyroid, testes, ovaries
- Macroscopic: all tissues (see microscopy) from all animals
- Microscopic: from all animals: skin, brain, lung, spleen, pancreas, stomach, small and large intestines, kidneys, urinary bladder, gallbladder, ovaries, testes, bone marrow,

heart, prefemorral and mesenteric lymphnodes, liver, adrenals, thyroid, parathyroid, eye, pituitary, sciatic nerve, spinal cord, thymus, skeletal muscle, gross lesions

STATISTICAL METHODS: ANOVA, Bartlett's test, t-test (Steel), Dunnett's test

Result : TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: one male at 10 mg/kg bw on day 20 and 3 females at 100 mg/ kg bw during week 3
- Clinical signs: In males at 100 mg/kg bw red swollen eye, ocular and/or nasal discharge were seen.
In animals that died diarrhoea was apparent on the day before death
- Dermal effects:
Skin effects were seen at all dose groups with increasing incidence and severity. At 1.0 mg/kg bw effects were restricted to erythema and oedema in all animals. At 10 mg/kg bw atonia and corisceousness were seen next to erythema and oedema. At 100 mg/kg bw fissuring of the skin and desquamation was seen in addition to erythema, oedema, atonia and corisceousness
- Body weight gain: no treatment related effects
- Haematology:
At 10 and 100 mg/kg bw the number of erythrocytes was increased in males. At 100 mg/kg bw an increased haemoglobin level was reported in males. Leucocyte counts were increased in males and females at 10 mg/kg bw and in males at 100 mg/kg bw
- Clinical chemistry:
BUN and ALAT were decreased in the surviving female at 100 mg/kg bw
- Urinalysis:
A decreased volume was reported in males at 1.0 and 100 mg/kg bw; specific gravity was increased at 1.0 mg/kg bw
- Organ weights:
Liver weight was decreased in females at 1.0 and 10 mg/ kg bw (both absolute and relative)
Relative spleen weight was decreased in mid and high dosed females
Absolute kidney weight and absolute and relative adrenal weight were decreased in females at 10 mg/kg bw
- Gross pathology:
Skin lesionss at the application site consisting of thickening, encrustation, sloughing, necrosis, leatherness, foci in the dermis and epidermis were reported in all treated animals
- Histopathology:
Skin effects (application site) included inflammatory cell infiltrate, acanthosis, hyperkeratosis and necrotic exudate on the epidermal surface at 1.0 mg/kg bw. At 10 and/or 100 mg/kg bw additionally dermal fibroplasia and ulceration was reported.
At 100 mg/kg hyperplasia of the lymphnodes was seen.
Other incidental findings included areas of asperm and ectatic tubuli in the testes, lung congestion, lymphoid infiltrate in the liver, meningitis, nodules in the brain, cysts in the thyroid.
Several animals showed an infection of coccidia in their small intestine

STATISTICAL RESULTS: Effects on RBC and HB and liver weight

reached a level of statistical significance

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Conclusion	:	Based on local effects the LOAEL is 1.0 mg/kg bw. For systemic effects a NOAEL of 100 mg/kg bw can be derived. The lymphnode hyperplasia was considered secondary to skin effects.
Reliability	:	(2) valid with restrictions 1 No analyses were performed to check the actual amount of test substance applied. 2 The number of animals/treatment was too small. Abrasion of the skin of half of the animals did not seem to influence the results, but is not requested by the OECD guideline 3 Effects on blood parameters remained within historical values. 4 The liver effects were only seen in females and showed no relationship with dose or microscopic changes. Therefore they were considerd to be not related to treatment.

13.12.2007 (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	HGPRT assay
System of testing	:	CHO-cells (K1-BH4)
Test concentration	:	62.5-250 ug/mL
Cycotoxic concentr.	:	200 ug/mL
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

SYSTEM OF TESTING
- Species/cell type: CHO-K1-BH4
- Proficiences: HGPRT
- Metabolic activation system: Arochlor-1254-induced male rat liver homogenate

ADMINISTRATION:
- Dosing: with and without S9 100, 125, 150, 200 and 250 ug/mL; additionally with S9 62.5 and 75 ug/mL
- Number of replicates: one
- Positive and negative control: 5-Bromo 2'deoxyuridine (-S9), 3-methylcholanthrene (+S9) and DMSO (vehicle)
Exposure time: 1.5E06 cells were exposed for 4 h followed by 6-7 day expression time

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Kastenbaum and Baumann

Result : GENOTOXIC EFFECTS:
- With metabolic activation: negative
- Without metabolic activation: negative

FREQUENCY OF EFFECTS: number of mutants remained within (negative) control ranges with the exception of the number of mutants in the lowest dose tested with S9-mix. Positive controls gave the expected results

PRECIPITATION CONCENTRATION: not observed

CYTOTOXICITY (% of control survival) at the highest tested concentration:
- With metabolic activation: 0.4% at 250 ug/mL
- Without metabolic activation: 20% at 250 ug/mL

STATISTICAL RESULTS: The increase of the number of mutants at 62.5 ug/mL (+S9) was statistically significant

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test substance : II, CAS 583-78-8 (2,5-dichlorophenol), purity >98%
Reliability : (2) valid with restrictions
1. The report is limited to the above mentioned.
2. The increased number of mutants seen at 62.5 ug/mL in the assay with metabolic activation is considered to be not relevant, since no concentration effect relationship was observed.

13.12.2007 (17) (18)

Type : Ames test
System of testing : Salmonella typhimurium TA100, TA1535, TA1537, TA98
Test concentration : 2 - 200 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year : 1983
GLP :
Test substance :

Method : The preincubation method was used. Metabolic activation was accomplished with S9 prepared from rat liver and hamster liver induced with Aroclor 1254.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

10.12.2007 (19)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : NMRI
Route of admin. : gavage
Exposure period : single dose
Doses : 1500 mg/kg bw
Result : negative
Method : other: not indicated
Year :
GLP : no data
Test substance : other TS

Method : TEST ORGANISMS:
- Age: 8-12 weeks
- Weight at study initiation: not indicated
- No. of animals: 10/treatment

ADMINISTRATION:
- Vehicle: corn oil

		- Frequency of treatment: single dose by oral gavage (volume 5 ml/kg) - Sampling times: 24, 48 and 72 hours after treatment (samples from 10 animals each time, number of bone marrow smears not indicated) - Control groups and treatment: negative: corn oil (5 ml/kg) positive: cyclophosphamide (20 mg/kg bw in deionised water) EXAMINATIONS: - % of polychromatic erythrocytes (PCE) in 1000 erythrocytes - Number of micronucleated PCE/1000 PCE CRITERIA FOR EVALUATING RESULTS: - Statistical method: Wilcoxon's non-parametric rank sum test
Result	:	TOXIC RESPONSE/EFFECTS BY DOSE LEVEL: Not reported EFFECT ON PCE/NCE RATIO: % PCE 44.6, 32.0 and 27.6 at 24, 48 and 72 hours, resp. GENOTOXIC EFFECTS: Mean number of micronucleated PCE: 0.6, 1.4 and 0.9 at 24, 48 and 72 hours sampling time, resp. STATISTICAL RESULTS: % PCE significantly decreased at the 72-hours sampling time
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity >98%
Conclusion	:	not clastogenic
Reliability	:	(2) valid with restrictions 1. The report was limited to the above mentioned. 2. The proportion of micronucleated PCE was determined for 1000 PCE. This is in agreement with OECD 474 (1983); OECD 474 (1997) requires evaluation of 2000 PCE.
13.12.2007		(17) (18)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

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IUCLID

Data Set

Existing Chemical	:	ID: 1918-00-9
Memo	:	TRA
CAS No.	:	1918-00-9
Generic name	:	2-methoxy-3,6-dichlorobenzoic acid
Synonym	:	3,6-dichloro-o-anisic acid
Product name	:	dicamba
Producer related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Substance related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	20.12.2007
Revision date	:	
Date of last update	:	20.12.2007
Number of pages	:	47
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	87 - 108 °C
Sublimation	:	
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	1981
GLP	:	yes
Test substance	:	other TS
Method	:	Test was performed according to OECD 102, capillary method - metal block apparatus. Two capillary tubes containing finely ground test substance were tested simultaneously (determination 1 and 2). Melting point of acetanilide was measured to determine the accuracy of the apparatus before the actual test.
Result	:	determination 1 determination 2 beginning of 87 87 melting (deg C) final stage of 108 108
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (dicamba, technical), purity 85.9% (by HPLC)
Conclusion	:	melting range is 87-108 deg C
Reliability	:	(1) valid without restriction No results for the reference substance are given. However, accuracy was estimated to be 0.5 deg C which is by far exceeded by the length of the temperature range.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

2.2 BOILING POINT

Value	:	ca. 329 °C at
Decomposition	:	
Method	:	other: estimated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using MPBWIN v1.01 in EPIWIN v3.20.
Result	:	---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 329.17 deg C (Adapted Stein and Brown Method) Melting Point: 213.41 deg C (Adapted Joback Method) Melting Point: 78.54 deg C (Gold and Ogle Method) Mean Melt Pt : 145.97 deg C (Joback; Gold,Ogle Methods) Selected MP: 112.26 deg C (Weighted Value) Vapor Pressure Estimations (25 deg C): (Using BP: 329.17 deg C (estimated)) (Using MP: 115.00 deg C (exp database)) VP: 3.15E-005 mm Hg (Antoine Method)

VP: 5.29E-005 mm Hg (Modified Grain Method)
VP: 0.000102 mm Hg (Mackay Method)
Selected VP: 5.29E-005 mm Hg (Modified Grain Method)
Subcooled liquid VP: 0.000262 mm Hg (25 deg,C, exp database VP)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-O- (nonring)	25.16	25.16
Group	1	-COOH (acid)	169.83	169.83
Group	2	CH (aromatic)	28.53	57.06
Group	4	-C (aromatic)	30.76	123.04
Group	2	-Cl (to aromat)	36.79	73.58
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		668.83
RESULT- corr		BOILING POINT in deg Kelvin		602.33
		BOILING POINT in deg C		329.17

Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Acceptable method of estimation.

13.12.2007 (2)

2.4 VAPOUR PRESSURE

Value : .0000167 hPa at 25 °C
Decomposition : ambiguous
Method : other (measured): US EPA Pesticide Assessment Guidelines (40 CFR 158), Subdivision D, No 63-9. Essentially OECD 104, gas saturation method.
Year :
GLP : yes
Test substance : other TS

Method : VP was determined at 8 different temperatures between 95 and 111 deg C using a Dupont 916 Thermal Evolution Analyzer. Using this apparatus, test substance saturation in a carrier gas is achieved at a certain temperature. The gas chamber effluent is swept to an on-line coupled Flame Ionization Detector, the response of which is proportional to the number of moles of TS reaching the detector per unit of time. TS (0.1061 g) was loaded on sea sand (0.9373 g). Nitrogen was used as carrier gas; VP was determined at 3 flow rates (0.680, 1.858 and 3.893 mL/min) for each temperature. Validity of the method was determined using dimethylphthalate as a reference substance.
VP at 25 deg C was determined by extrapolation of a log VP vs. 1000/T line.
Remark : The vapor pressure is supported by the EPIWIN v3.05 calculated value of 0.0000075 hPa.
Result : Temperature (deg C) / Average empirical VP (mm Hg)

Temperature (deg C)	Average empirical VP (mm Hg)
95	0.1080
97	0.1281
99	0.1500
100	0.1796
104	0.2558

	106	0.3209
	110	0.4512
	111	0.5471

Log VP = -6145.6/T (K) + 15.7189 (mm Hg)
with T(K) = t(deg C) + 273
(correlation coefficient = -0.9980)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (dicamba), purity 99.18% (HPLC)
Conclusion VP at 25 deg C = 1.25E-5 mm Hg (1.67E-5 hPa)
Reliability : (2) valid with restrictions
Extrapolation from 95 deg C as lowest T to 25 deg C may cause a relative error since, at 95 deg C TS may be partially fluid, whereas at 25 deg C it is a solid. Extrapolation may therefore be problemetic. It is, however, the best possible option under these circumstances.
Flag : Critical study for SIDS endpoint
25.12.2001 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = 2.21 at °C
pH value :

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Score of 2 given to handbook or published values for physical constants. The measured value in the other listed study is for the partially ionized form of the TS.
Flag : Critical study for SIDS endpoint
25.12.2001 (4)

Partition coefficient :
Log pow : .545 at 25 °C
pH value :
Method : other (measured): EPA Pesticide Assessment Guidelines, Subdivision D, Product Chemistry, Section 63-11. Essentially OECD 107
Year : 1982
GLP : yes
Test substance : other TS

Method : Because test substance dissociates in aqueous and octanol phase, Kow of non-dissociated TS was calculated on basis of measured test substance concentrations and pH of the two phases and on pKa of the test substance (1.94).

0.497 mg and 5.054 mg test substance (specific activities 1.28E6 dpm/mg and 1.26E5 dpm/mg, respectively) were each dissolved in 5 mL buffer-presaturated n-octanol after which 5 mL n-octanol-presaturated buffer was added. The mixtures were shaken in a water bath at 25 deg C for 1 hour, centrifuged (2000 rpm, 20 min) and duplicate 1.0 mL aliquots were taken from both phases and analyzed by LSC. The pH of each phase was measured.
Three buffer solutions of pH 5.0, 7.0 and 9.0 were used. For each pH and each TS concentration triplicate test mixtures were prepared.
The fraction of undissociated dicamba in each phase was

calculated on basis of measured ion concentration, pKa and pH.

Result : Buffer pH Initial TS concentration in n-octanol (mM) Kow (mean of 3 replicates)

5.0	4.58	6.86 +/- 0.60
7.0	4.58	0.54 +/- 0.01
9.0	4.58	8.95 +/- 0.06
5.0	0.499	3.98 +/- 0.11
7.0	0.499	0.16 +/- 0.00
9.0	0.499	0.58 +/- 0.00

Average Kow: 3.51 +/- 3.73

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba), analytical reference standard
I, CAS 1918-00-9 (14C-dicamba), radiochemical purity 98%

Conclusion : Kow of test substance strongly depends on pH and on test substance concentration.
Kow ranged between 0.2 and 9.0.

Reliability : (2) valid with restrictions
1. Measurement was performed on ionized form of TS, which results in deviations from the partition law. Measurement should have been performed on non-ionized TS and therefore at low pH. OECD 107 suggests pH at least one unit below pKa. However, as pKa = 1.94 pH should have been < 1 which is very low. Therefore, this has to be considered best possible method.
2. Only one n-octanol: water ratio was tested for each pH and concentration.

25.12.2001 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in :
Value : 8.24 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : soluble (1000-10000 mg/L)
Stable :
Deg. product :
Method : other: essentially OECD 105 (flask method)
Year : 1993
GLP : yes
Test substance : other TS

Method : 25 mL water of Milli-Q reagent grade were added to 0.50 g test substance. The mixture was shaken for about one hour and was then placed in a water bath (25 deg C) for at least 48 hrs. With intervals of at least 24 h the mixture was centrifuged and returned to a waterbath (25 deg C) for temperature equilibration (at least 1 h). The test solutions were analyzed in duplicate using HPLC against dicamba calibration standards (dicamba in methanol, 1.028-10.285 mg/mL). Measurements were repeated until SD of the two last

measurements was within the method reproducibility.

Remark	:	This value is supported by a vlaue of 6500 mg/L at 25 C given by: Tomlin, C.D.S. (ed.). The Pesticide Manual - World Compendium. 10th ed. Surrey, UK: The British Crop Protection Council, 1994. 298 (as cited in Hazardous Substance Data Base)
Result	:	Solubility in water at 25 deg C: 0.824 g per 100 mL solution
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (dicamba, technical), purity 85.9%
Conclusion	:	Solubility of test substance in water is 8.24 g/L.
Reliability	:	(2) valid with restrictions 1. Only the end result is reported, no individual results of measurements are given. Results can therefore not be checked. 2. Method is intended for essentially pure chemicals. Dicamba technical cannot be regarded as such. 3. It should be noted that whereas technical dicamba was tested, a reference standard of 99.18% purity was used for calibration. Impurities have therefore been disregarded.
Flag	:	Critical study for SIDS endpoint

25.12.2001 (6)

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Xenon lamp
Light spectrum	:	> 290 nm
Relative intensity	:	1.32 based on intensity of sunlight
Conc. of substance	:	100.19 mg/l at 25 °C
DIRECT PHOTOLYSIS		
Halflife t1/2	:	50.3 day(s)
Degradation	:	31.3 % after 30 day(s)
Quantum yield	:	
Deg. product	:	yes
Method	:	EPA Guide-line subdivision N 161-2 "Photodegradation studies in water"
Year	:	1982
GLP	:	yes
Test substance	:	other TS

Method :

A 1000 mL test solution consisting of 100.19 mg dicamba with a specific activity of 412.2 dpm/ug (total 688 kBq) in aqueous buffer solution pH 7 containing 1% acetonitrile was prepared. The test solution was incubated at 25 +/- 1 deg C under contineous stirring for 30 days. Average incident radiation on the reactor surface was 7.704E2 W/m2 (measured before and after the study).
The reaction solution was aerated and connected to a silica gel trap, an ethylene glycol trap (organic volatiles) and a 10% NaOH trap (supposed to collect CO2) in series. Before initiation of photolysis, a 50 mL sample was taken as dark control sample. 20 mL samples were taken before initiation of photolysis and on day 1, 3, 8, 15, 22 and 30.

The samples were analyzed as follows:
- duplicate 1 mL samples were analyzed by LSC
- 15 mL was extracted twice at pH < 1 with ethyl acetate, both fractions were analyzed by LSC (duplicate 1 mL samples)
- ethyl acetate fraction was dried and concentrated, and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- extracted buffer solution of day 15, 22 and 30 were lyophilized followed by acetonitrile extraction; the extract was concentrated and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- duplicate 1 mL ethylene glycol and 10% NaOH trap samples were analyzed by LSC
- silica gel traps were extracted with with methanol, which was then analyzed by LSC; residual radioactivity in the silica traps was determined by combustion
- identity of radioactivity supposed to be CO2 in 10% NaOH trap samples was confirmed for day 22 and 30 by precipitation as BaCO3 and subsequent evolution as CO2 after addition of HCl

On day 30, the reactor was washed with methanol and with acetone. Volumes were measured and 1 mL duplicatealiquots were analyzed by LSC.

Photodegradation was calculated using the SAS Regression Program.

Result : time point (days) 14C-dicamba (% of actually applied

14C-dicamba)*

0	100 (92.14% of applied 14C)
1	98.83
3	95.25
8	86.87
15	75.62
22	66.44
30	58.74 (degradation: 41.26%)
30 (dark control)	98.61

* calculated by reviewer from % of applied 14C
Unchanged dicamba was confirmed by HPLC.

All other compounds in the different fractions, separated by TLC, were <10% of applied 14C and did not match with reference standards. CO2 in the 10% NaOH trap was 11.7% of applied at day 22 and 16.6% of applied 14C at day 30. Radioactivity in the other traps was <10% of applied 14C at all time points. Reactor wash yielded 0.3% of applied activity. The mass balance was >99% and <103.5% at all time points.

Under these conditions, t1/2 of dicamba was 38.1 days; the photolysis rate constant was 0.018 day-1. Based on the spring sunlight intensity at 40 deg latitude at noon (5.83E2 W/m2) the corresponding photodegradation rate for natural sunlight will be 0.0138 day-1; t1/2 will be 50.3 days.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (dicamba), purity 99.6% by IR
I, (14C-dicamba), radiochemical purity 100% by TLC
Conclusion : The photodegradation rate constant in spring sunlight at 40 deg latitude at noon is 0.0138 day-1; t1/2 is 50.3 days. The major photodegradation product is CO2.
Reliability : (1) valid without restriction
1. In the calculation of t1/2, no correction for the degradation in the dark control was made. However, this will only slightly influence the results, as there was hardly any degradation in the dark control.
2. Except for sterilization of the buffer solution, no measures to guarantee sterility of the samples were described. However, as there was hardly any degradation in the dark control (which was a subsample of the sample to be irradiated), it can be assumed biodegradation was negligible.
Flag : Critical study for SIDS endpoint
25.12.2001 (7)

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : ca. .000000000002895 cm³/(molecule*sec)
Degradation : % after
Deg. product :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Method : Estimation using AOP Program v1.92 in EPIWIN v3.20.
Result : AOP Program (v1.92) Results:
==========
SMILES : COc1c(CL)ccc(CL)c1C(=O)(O)
CHEM : Dicamba
MOL FOR: C8 H6 CL2 O3
MOL WT : 221.04
-------- SUMMARY (AOP v1.92): HYDROXYL RADICALS --------
Hydrogen Abstraction = 0.8296 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.5200 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 1.6354 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 2.9850 E-12 cm3/molecule-sec
HALF-LIFE = 3.583 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 42.999 Hrs
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi): 0.00496 (Junge,Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation
Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Acceptable method of estimation.

13.12.2007 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Degradation : = 0 - 7.6 % after 30 day(s) at pH and °C
Deg. product :
Method : other: essentially OECD 111
Year : 1981
GLP : no
Test substance :

Method : Solutions of 10 ppm and 100 ppm dicamba (1.17% and 0.12% 14C-dicamba, respectively) in distilled water or aqueous buffer solutions of pH 5.0, 7.0 and 9.0 were incubated at 25 and 35 deg C for 30 days (volume 201 mL, in amber bottles in shaking water baths). Acetone concentrations were 0.5%. After 1, 7, 14, 21 and 30 days, a duplicate 1-mL sample was taken for radioassay and a duplicate 15-mL sample was taken for extraction using diethyl ether (at pH < 1). Organic and aqueous layers were first radioassayed and then analyzed using TLC and radioautography detection, followed by quantification using LSC. Samples were cochromatographed with dicamba and three metabolite reference standards.
Result : There was no significant dicamba hydrolysis (i.e. equal to or less than 7.6%) at each pH value, both concentrations and both temperatures, except for 100 ppm, pH 7.0, 35 deg C at

t=14, 21 and 30 days in the 100 ppm, when degradation was up to 18.5%. Total recovery was only 82.5-83.4% for these samples, whereas it was > 95 for all other samples. Radioactivity remaining in the aqueous phase after extraction was equal to or less than 1% of applied. Three unknown degradation products each constituted less than 4% of applied.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (14C-dicamba), purity not specified
I, CAS 1918-00-9 (14C-dicamba), radiochemical purity greater than 98%

Conclusion : Dicamba is stable with slight or no hydrolysis over 30 days under the conditions tested.

Reliability : (2) valid with restrictions
1. The fact that at 100 ppm, pH 7.0, 35 deg C up to 18.5% degradation occurred was disregarded because recoveries were low. However, no explanation was given for the low recoveries. It cannot be excluded that loss of radioactivity is due to hydrolysis.
2. Section "Results and discussion" contained 2 values that were not in agreement with values in tables of results.
3. No measures to guarantee sterility of the samples or to exclude oxygen from the solutions were described. However, as measured degradation percentages were very low (except at 100 ppm, pH 7.0, 35 deg C), no significant biotic degradation or oxidation can have occurred.
2. No duplicate samples at any pH.
3. pH 5.0 was tested, whereas OECD 111 prescribes pH 4.

25.12.2001 (8)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: estimated
Year :

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN v3.20. An experimental melting point range of 87-105 deg C was previously determined; the average of these values (97.5 deg C) was used in the fugacity calculations. Equal emissions to air, water, and soil were assumed. Other parameters used the default values found in EPIWIN.

Result : Level III Fugacity Model (Full-Output):

==========

Chem Name : Dicamba
Molecular Wt: 221.04
Henry's LC : 2.18e-009 atm-m3/mole (Henry database)
Vapor Press : 8.09e-005 mm Hg (Mpbpwin program)
Liquid VP : 0.000422 mm Hg (super-cooled)
Melting Pt : 97.5 deg C (user-entered)
Log Kow : 2.21 (Kowwin program)
Soil Koc : 66.5 (calc by model)

	Mass Amount	Half-Life	Emissions

	(%)	(hr)	(kg/hr)
Air	0.0194	86	1000
Water	19.6	900	1000
Soil	80.2	1.8e+003	1000
Sediment	0.0999	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	9.7e-013	7.09	8.8	0.236	0.293
Water	4.4e-014	687	892	22.9	29.7
Soil	1.05e-012	1.4e+3	0	46.8	0
Sediment	4.31e-014	0.388	0.0908	0.0129	0.00303

Persistence Time: 1.51e+003 hr
Reaction Time: 2.17e+003 hr
Advection Time: 5.04e+003 hr
Percent Reacted: 70
Percent Advected: 30

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 85.99
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.327 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
13.12.2007 (2)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic
Concentration : 100 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : = 5 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 5 day(s) < 6 %
11 day(s) = 5 %
15 day(s) = 5 %
20 day(s) = 5 %
28 day(s) = 5 %
Control substance : Acetic acid, sodium salt
Kinetic : 11 day(s) = 87 %
28 day(s) = 87 %
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 2001
GLP : yes
Test substance : other TS

Method : Methods were carried out in accordance with OECD Method 301F, Manometric Respirometry. Two experimental controls were run in this experiment. Inoculum blanks included viable organisms without test substance to ensure that no additional carbon source existed for the organisms. Abiotic controls were run in which the organisms were killed by the addition of HgCl2, ensuring the presence of the test substance in a medium that contained the same amount of particulate matter as the test bottles. A toxicity control (test substance, reference compound, and inoculum), as specified under 301F, was not run. The test medium and apparatus were created in accordance with OECD and EU guidelines. The test organisms were obtained from a domestic sewage treatment plant and were maintained at a neutral pH in aerobic conditions. Blank controls and test substance bottles were prepared in triplicate along with six reference compound bottles. Oxygen uptake was measured on weekdays during the 28 day period and reported on days: 5, 11, 15, 20, and 28.

COD was determined using the UK Department of the Environment method. A COD value of 0.69 gO2/g was obtained experimentally for sodium acetate and a value of 1.04 gO2/g was obtained for the test substance. These values were used in the calculations for each respective compound. Biodegradation was calculated as BOD divided by COD multiplied by 100%. This was done instead of ThOD, as COD is a more accurated indication of the maximum oxygen demand of the reference compound, sodium acetate.

Result : The BOD value for the test substance was 5%, which indicates that it is not readily biodegradable. For the reference compound, a maximum biodegradation of 87% was observed.

Test condition : The pH of the test flasks were kept near neutral to not bias oxidation or reduction potentials. The tests were performed at 22C +/- 2C.

Test substance : The test substance, SAN837A, Batch Sample Ref. P.MG2726410, (3,6-dichloro-2-methoxybenzoic acid, CAS number 1918-00-9), commonly known as Dicamba, was assigned the Brixham test substance ID of AJ0222. A certificate of analysis stated that the test substance had a purity of 89.9%. The sample was stored in the dark and at ambient temperature unti the beginning of the experiment.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

15.10.2007 (9)

Remark : Dicamba has a half life of 31 days with a first-order rate constant of 0.0224/day in a typical midwestern agricultural soil under aerobic conditions. Dicamba is completely mineralized to CO2 under aerobic conditions with 3,6-dichlorosalicylic acid as the only major metabolite. Low levels of 2,3-dihydroxy-3,6-dichlorosalicylic acid were detected. Metabolism under anaerobic conditions is similar to that which occurred in aerobic soil except the rate of dicamba metabolism is reduced under anaerobic conditions. [Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

AQUATIC FATE: Based on the results of various studies, microbial degradation appears to be the important dicamba removal process in natural water. Photolysis may contribute to dicamba removal from water(Scifres CJ et al; J Environ Qual 2: 306 (1973) As cited in HSDB update of 8-09-2001.

Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9 (dicamba)

Conclusion : Although not readily biodegradable, evidence exists to indicate that dicamba can biodegrade under both aerobic and anaerobic conditions.

12.12.2007

05.10.2007

05.10.2007

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	= 56 measured/nominal
LC50	:	= 134.5 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	other: Committee on Methods for Toxicity Tests with Aquatic Organisms, 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009
Year	:	1975
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Species: Salmo gairdneri Richardson (Rainbow trout)
- Supplier: Cultured in Union Carbide Environmental Services Laboratory from eggs obtained from a commercial hatchery.
- Size: Mean length of 37 mm, mean weight of 0.36 g, age = 4 months
- Biological loading: 0.24 g/L
- Acclimation to test dilution water: 24 hours prior to testing
- Feeding: discontinued 48 hours prior to test. Not fed during test

TEST SOLUTION PREPARATION:
Stock solution of the test material was prepared in acetone. The amount of solvent in the solvent control equalled the amount used in the highest test concentration but was not stated.

DILUTION WATER:
- Reconstituted soft water, pH of 7.26, total hardness of 42 mg/L as CaCO3, total alkalinity of 29 mg/L as CaCO3, specific conductance of 149 umhos/cm.

TEST SYSTEM:
- Static test
- Concentrations: Control, Solvent Control, 18, 32, 56, 100 and 180 mg/L (nominal)
- Exposure vessels: 5 gallon glass jars containing 15 L of dilution water
- Number of fish: 10 per treatment
- Temperature: 12 degrees C +/- 1
- Photoperiod: not indicated

PHYSICAL MEASUREMENTS:
- Dissolved oxygen and pH determined at 0, 48 and 96 hours in the control, solvent control, low, medium and high test concentrations. Temperature determined at 0 and 96 hours in same vessels.

- DO: 9.5 - 10.2 mg/L at 0 hours, 8.0 - 9.8 mg/L at 96 hours
- pH: decreased with increasing test concentration. At 180 mg/L, initial pH = 5.92, final pH = 4.09.
- Temperature: 12 degrees C +/- 1

BIOLOGICAL MEASUREMENTS:
- Mortality and abnormal behavior noted at 24, 48, 72 and 96 hours

STATISTICAL ANALYSES:

- LC50 determined by Speaman-Karber estimator (Finney, 1971) based upon mortality at 48 and 96 hours.
- NOEC based upon abnormal behavior at 96 hours.

Remark : Additional data are available for bluegill sunfish (Lepomis machrochirus) in which the 96-hour LC50 was determined to be 112 mg/L (1) and 136.3 mg/L (2).

(1) Acute Toxicity of Banvel XP to Bluegill (Lepomis macrochirus), EG&G Bionomics, Inc., June 1974, prepared for Velsicol Chemical Corp., BASF 1974/5158;
(2) The Acute Toxicity of Banvel Technical to the Bluegill Sunfish (Lepomis macrochirus) Rafinesque, Union Carbide Environmental Services, December 1977, prepared for Velsicol Chemical Corp., BASF 1977/5075.

Result : Rainbow trout exposed to concentration of 100 mg/L and higher exhibited surfacing behavior up to 72 hours. At 96 hours, these fish appeard normal. The NOEC was 56 mg/L based upon these observations.

No mortality was observed at concentrations up to and including 100 mg/L at any time period. All fish exposed to 180 mg/L were dead at the 48 hour observation period.

The 48-hour and 96-hour LC50 are both = 135.4 mg/L. Confidence intervals could not be obtained due to the lack of partial mortalities.

Test substance : Banvel Technical, 86.82%, lot no. 52625110

Reliability : (2) valid with restrictions
Test performance was checked against EPA OPPTS 850.1075 (1996).
- Analytical confirmation of test concentrations was not performed.
- No mention of photoperiod.
- Concentration of solvent used was not specified.
- pH values in the highest test concentration were outside the recommended range of 6.0 - 8.5, but this was due to properties of the test material.

Flag : Critical study for SIDS endpoint
06.12.2007 (10)

Type : static
Species : Cyprinodon variegatus (Fish, estuary, marine)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > 180
Limit test :
Analytical monitoring : no
Method : other: EPA-660/3-75-00
Year : 1975
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Species: Cyprinodon variegatus
- Supplier: commercial supplier in Florida
- Size (mean)/weight (mean)/loading: 32 mm/480 mg/0.32 g/L
- Feeding (pretreatment): discontinued 48 hours prior to test
- Feeding during test: none

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: acetone
- Concentration of vehicle/ solvent: < 0.5 mL/L

DILUTION WATER
- Source: artificial seawater (origin well water)
- Chemistry (Salinity;pH): 27 ppt; 8.18

TEST SYSTEM
- Test type: static
- Concentrations: 18, 32, 56, 100 and 180 mg/L, solvent treated and untreated controls
- Exposure vessel type: 20 L glass vessel containing 15 L water
- Number of fish: 10/treatment
- Photoperiod: not indicated
PHYSICAL MEASUREMENTS
- Measuring times: 0, 48 (only O2), 96 h in controls, 18, 56 and 180 mg/L
- Dis. oxygen: 101-104% (0 h), 74-83% (48 h), 51-78% (96 h)
- pH: 7.5-8.2, for 180 mg/L 6.6-7.4
- Test temperature: 21 C

DURATION OF THE TEST: 96 hours

TEST PARAMETER: Mortality
OBSERVATION TIMES: 24, 48 and 96 hours

STATISTICAL METHOD: not applicable

Result : RESULTS:
- Mortality: no mortality
- Other effects: not reported

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba technical), purity 86.82%

Reliability : (2) valid with restrictions
Test performance was checked against EPA OPPTS 850.1075 (1996):
A) No analyses were performed to confirm the nominal test concentrations (EPA >80% of nominal)
B) The dissolved oxygen concentration was lower than recommended in some test vessels at the end of the test only (51-78% at 96 hours, EPA >60%); the salinity was higher than recommended (27 ppt, EPA 20 +/- 5 ppt);
pH-values in the highest tested concentration only were lower than recommended (6.6-7.4, EPA 7.5-8.5), due to inherent properties of the test substance; the photoperiod was not indicated (EPA 12-16 h light).

06.12.2007 (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : = 56 measured/nominal
EC50 : = 110.7 measured/nominal
Analytical monitoring : no
Method : other: Committee on Methods for Toxicity Tests with Aquatic Organisms, 1975, Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians, EPA-660/3-75-009
Year : 1975
GLP : no
Test substance : other TS

Method : TEST ORGANISMS:
- Species: Daphnia magna Straus
- Supplier: Cultured in Union Carbide Environmental Services Laboratory

- Age: Less than 20 hours old
- Acclimation to test dilution water: Gravid adults isolated in dilution water 20 hours prior to testing

TEST SOLUTION PREPARATION:
A primary stock solution of the test material was prepared in acetone and a secondary stock prepared by serial dilution. The amount of solvent in the solvent control equalled the amount used in the highest test concentration but was not stated.

DILUTION WATER:
- Filtered lake water, pH of 7.34, total hardness of 50 mg/L as CaCO3, total alkalinity of 32 mg/L as CaCO3, specific conductance of 150 umhos/cm.

TEST SYSTEM:
- Static test
- Concentrations: Control, Solvent Control, 18, 32, 56, 100 and 180 mg/L (nominal)
- Exposure vessels: 250 mL glass beakers containing 200 mL of test solution. Four replicate beakers per treatment.
- Number of Daphnids: 5 per beaker (20 per treatment)
- Temperature: 18 degrees C +/- 1, maintained in a water bath
- Photoperiod: not indicated

PHYSICAL MEASUREMENTS:
- Dissolved oxygen and pH determined at 0 and 48 hours in the control, solvent control, low, medium and high test concentrations.

- DO: 8.6 - 9.0 mg/L at 0 hours, 8.4 - 8.9 mg/L at 48 hours
- pH: decreased with increasing test concentration. At 180 mg/L, initial pH = 3.62, final pH = 3.66.
- Temperature: 12 degrees C +/- 1

BIOLOGICAL MEASUREMENTS:
- Mortality recorded at 24 and 48 hours

STATISTICAL ANALYSES:
- LC50 determined by Speaman-Karber estimator (Finney, 1971) based upon mortality at 48 hours.

Remark : Results reported as LC50 (mortality) rather than EC50 (immobility).

Result : At 48 hours, mortality was 30% at 100 mg/L and 100% at 180 mg/L. Mortality of 5% was noted at 18 mg/L, but was not considered test-substance related, since there was no mortality at the next two higher concentrations. The NOEC was 56 mg/L based upon mortality.

The 24-hour LC50 was reported as 120.7 mg/L (95% confidence interval 108.0 - 134.8 mg/L).

The 48-hour LC50 was reported to be 110.7 mg/L (95% confidence interval 96.8 - 126.6 mg/L).

Test substance : Banvel Technical, 86.82%, lot no. 52625110

Reliability : (2) valid with restrictions
Test performance was checked against EPA OPPTS 850.1010 (1996).
- Analytical confirmation of test concentrations was not performed.
- No indication that test temperature was measured during the test.
- No mention of photoperiod.
- Concentration of solvent used was not specified.
- pH values in the highest test concentration were outside the recommended range of 6.0 - 8.5, but this was due to properties of the test material.

Flag : Critical study for SIDS endpoint

06.12.2007 (12)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: cell counts
Exposure period	:	120 hour(s)
Unit	:	mg/l
NOEC	:	3.7
EC0	:	3.7
EC10	:	> 3.7
EC50	:	> 3.7
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: EPA FIFRA 122-2, 123-2
Year	:	1982
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS
- Species: Selenastrum capricornutum, strain 1648, family Chlorophyceae
- Source/supplier: Carolina Biological Supply Company, Burlington, North Carolina
- Laboratory culture: stock culture at Springborn Laboratories
- Culturing: stock cultures were grown in 125 mL glass flasks containing 50 mL test medium and were transferred to fresh medium ~twice weekly.
- Pretreatment: at least 2 days prior to test initiation algae were maintained under test conditions (culture medium, 100 rpm, 25 C, continuous illumination (3200-4300 lux)
- Initial cell concentration: 0.3 E4 cells/mL

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

GROWTH/TEST MEDIUM CHEMISTRY
- MBL medium used
- Chemistry (Hardness (Mg+Ca) 0.4 mmol/L;TOC 2.1 mg/L;P 1.6 mg/L;N 14 mg/L;EDTA 12E-2 mmol/L)
- pH: 7.5 (after adjustment)

TEST SYSTEM
- Test type: static
- Concentrations: 4 mg a.i./L and controls
- Exposure vessel: 125 mL erlenmeyer flasks containing 50 mL of test medium (shaken at 100 rpm)
- Number of replicates: 3
- Photoperiod (intensity of irradiation): continuous (3200-4800 lux)

PHYSICAL MEASUREMENTS
- Measuring times: 0 and 120 h
- Test temperature: 25 C
- pH: 7.3-7.5 (0 h); 10.4 (120 h)

DURATION OF TEST: 120 hours

TEST PARAMETER: algal growth (cell counts), measured by a haemacytometer
OBSERVATION TIMES: 0, 24, 48, 72, 96, 120 h

ANALYSES:
- Method: direct HPLC-UV
- Sampling times: 0 and 120 h

STATISTICAL METHOD: t-test

Result : RESULTS:
- Nominal concentrations (mg a.i./L): 0, 4
- Measured concentrations (mg a.i./L): <LOQ, 3.7 (=93% of nominal)
- Cell density data after 0, 24, 48, 72, 96 and 120 h (x E4 cells/mL) :
0: 0.3, 3, 18, 39, 54, 258
4: 0.3, 3, 17, 44, 51, 260

GROWTH IN CONTROL: increased by a factor of 130 after 72 hours

ANALYTICAL RESULTS: validated at 0.025-2.5 mg/L (recovery 101+/-2%, LOQ 14 ug/L. QCs fortified at 4 mg/L showed a recovery of 83-119%.

STATISTICAL RESULTS: no significant differences between control and treatments

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (Dicamba technical), purity 89.5%

Reliability : (1) valid without restriction
Minor remark. The test medium was not in accordance with OECD 201. The pH-increase observed during the test was probably associated with the strong cell growth (factor 130 after 72 hours).

06.12.2007 (13)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1465 mg/kg bw
Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: corn oil
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: not specified - Age: not specified - Number: 5/sex/dose - Weight at study initiation: 200-248 g - Controls: no ADMINISTRATION: - Doses: 500, 794, 1250, 1984, 3150 and 5000 mg/kg bw - Doses per time period: single - Volume administered: 10 ml/kg bw for all dosage levels except for the 5000 mg/kg level where 20 ml/kg bw was administered. - Post dose observation period: 14 days - food was withheld overnight EXAMINATIONS: for mortality (at least daily). BODY WEIGHT: at dosing and at 14 days. STATISTICAL METHOD: Thompson (1947)
Result	:	MORTALITY: - Number of deaths at each dose: 500, 794, 1250, 1984, 3150, 5000 mg/kg bw 0/10, 1/10, 4/10, 4/10, 10/10, 10/10 - Time of death: within 48 hours after dosing CLINICAL SIGNS: no data on decendents BODY WEIGHT: all surviving rats exhibited normal body weight gains during the observation period NECROPSY FINDINGS: no data POTENTIAL TARGET ORGANS: no data SEX-SPECIFIC DIFFERENCES: LD50 males= 1879 mg/kg bw LD50 females= 1581 mg/kg bw
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion	:	LD50 1707 mg/kg bw = 1465 mg a.i./kg bw
Reliability	:	(2) valid with restrictions

1. The information was essentially confined to what is included in the current summary.
2. no data were presented for effects other than mortality.
3. The dose volume used at the 5000 mg/kg bw was higher than recommended (20 ml/kg, OECD 401 =< 10 ml/kg). Since at 3150 mg/kg all rats died already, the reliability is not lowered because of this.

04.04.2001 (14)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 8.2 mg/l
Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: no vehicle
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not specified
- Age: not specified
- Weight at study initiation: 206-245 g
- Number of animals: 5/sex/dose
- Controls: no

ADMINISTRATION:
- Type of exposure: whole body exposure to dust of test material
- Exposure duration: 4 hours
- Concentrations(nominal/measured): approx. nominal conc. of 9.6 mg/l or 8.2 mg a.i./l
- Particle size: not specified
- Type or preparation of particles: control by Wright Dust Feeder
- Air changes: no data

EXAMINATIONS: during exposure: changes in behavior and appearance, after exposure: pharmacodynamic and/or toxic signs; 14 days observation period

BODY WEIGHTS: not specified

ANALYSES:
- Method: no data
- Sampling times: no data

STATISTICAL METHOD: no data

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: during exposure: increased, then decreased motor activity, and nasal porphyrin discharge. 14 day observation period decreased motor activity (1/10), corneal

opacity (few rats).

BODY WEIGHTS: gains were normal during the study.

NECROPSY FINDINGS: no data

POTENTIAL TARGET ORGANS: no data

SEX-SPECIFIC DIFFERENCES: no data

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion	:	LC50 > 9.6 mg/l = > 8.2 mg a.i./l
Reliability	:	(2) valid with restrictions 1. The information was essentially confined to what is included in the current summary 2. As this is a limit test, the LC50 value was derived by the reviewer. 3. no individual data were present.

04.04.2001 (14)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 1716 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	other: not specified
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not specified
- Age: not specified
- Weight at study initiation: 2324-2454 g
- Controls: no

ADMINISTRATION:
- Area covered: not specified
- Occlusion: yes
- Vehicle: not specified
- Concentration in vehicle: not specified
- Total volume applied: not specified
- Doses: 2000 mg/kg bw
- Removal of test substance: washed with tepid tap water after 24 hours

EXAMINATIONS: observed for mortality over 14 days.

BODY WEIGHT: pre-dosing and at day 14

STATISTICAL METHOD: not specified

Result : MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: not specified

BODY WEIGHTS: normal gains during study period

NECROPSY FINDINGS: no data

POTENTIAL TARGET ORGANS: no data

SEX-SPECIFIC DIFFERENCES: no data

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion : LD50 > 2000 mg/kg bw = > 1716 mg a.i./kg bw
Reliability : (4) not assignable
1. The information was essentially confined to what is included in the current summary.
2. As this is a limit test, the LD50 value was derived by the reviewer.
3. Only 4 animals were used (OECD 402 5) of which 2 had an abraded skin, which could alter the permeability of the test substance.
4. no individual data were present.

04.04.2001 (14)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : oral feed
Exposure period : 13 weeks
Frequency of treatm. : in feed
Post exposure period : 4 weeks (subgroups)
Doses : Control
500 ppm (40.1 mg/kg/day males; 43.2 mg/kg/day females)
3000 ppm (239 mg/kg/day males; 266 mg/kg/day females)
6000 ppm (479 mg/kg/day males; 535 mg/kg/day females)
12000 ppm (1000 mg/kg/day males; 1065 mg/kg/day females)

Control group : yes, concurrent no treatment
NOAEL : = 6000 ppm
LOAEL : = 12000 ppm
Method : OECD Guide-line 408 "Subchronic Oral Toxicity - Rodent: 90-day Study"
Year : 1981
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
Wistar rats, 10 males and 10 females per group with an additional 10 males and 10 females in control and high dose groups for recovery. Animals were acclimated for 14 days and were approximately 6 weeks old at start of treatment. The range of body weight at study initiation was within 20% of the mean value for each sex.

TEST CONDITIONS:

Animals were housed 3 or 4 per cage, Macrolon cages with solid bottoms.
Feed and water ad libitum.
Temperature 23 C +/- 2 degrees
Air changes approx. 8 +/- 2 per hour
Relative humidity 55 +/- 25%
Photoperiod 12:12

OBSERVATIONS:
Clinical signs and mortality: checked twice daily except once daily on weekends. Detailed health check weekly.
Eyes were examined before treatment and before scheduled sacrifice in the control and high dose groups, and also in females in the intermediate dose group and during week 17 in the female recovery groups.

Animals were weighed and food consumption determined weekly. Test substance intake was calculated for each cage using mean bodyweight and food consumption data and the nominal dietary test material concentration.

Clinical pathology: During weeks 12 and 17 (recovery subgroups), samples of blood and urine were collected from all animals for haematology, blood chemistry, and urinalysis.

Following 13 weeks of treatment, all surviving animals from the main subgroups were sacrificed. All animals from the recovery subgroups were offered control diet for a 4-week recovery period and sacrificed at 17 weeks.

All animals were subjected to a full macroscopic evaluation post-mortem. The following organs were removed and weighed: liver, spleen, kidneys, adrenals, ovaries, testes, heart and brain. Tissue samples from all major organs and systems were preserved and examined for all control and high dose animals. Tissues from the lung, liver, kidneys and all abnormalities were also examined in all other animals.

DATA ANALYSIS:
ANOVA followed by Dunnett's test was performed on parametric data. For non-parametric data, Kruksal Wallis followed by Mann-Whitney-U was used. Count data were subjected to Chi-square followed by Fisher's exact test.

Result **:** Analysis of the diet showed that adequate exposure was obtained. Animals used in a background health check demonstrated the suitability of the test organisms.

MORTALITY AND CLINICAL SIGNS:
No deaths occurred. From the start of treatment, males and females at the highest dose showed clinical signs of reduced activity and slowed movement which for some animals continued to the end of the treatment period. Animals in this group were cold to the touch during the first 4 weeks. The behavior and appearance of males and females at the other doses was indistinguishable from the controls.

OPTHALMOSCOPY:
At the week 12 examination, females at the highest dose had a higher incidence of thin retinal blood vessels. Although probably due to the combined effect of bodyweight gain deficit and blood sampling, the relationship of this change to the test substance cannot be excluded. At the end of the recovery period, these differences were absent.

BODYWEIGHT CHANGE:
From the start of treatment, a statistically significant lower rate of bodyweight gain was recorded in animals of both sexes at 12000 ppm. The

deviation from control was 28% for males and 40% for females. This was reversed during the recovery phase although the weight difference between the groups was not eliminated.

FOOD CONSUMPTION:
From the start of treatment, statistically significantly lower food intakes were recorded for males and females at 12000 ppm. During the recovery period, males consumed a similar quantity of food as controls while previously treated females consumed more than the controls. Food intakes at the other dose levels were unaffected.

FOOD CONVERSION RATIO:
Animals treated at 12000 ppm had a less efficient utilization of food.

CLINICAL PATHOLOGY:
Significantly lower platelet count and partial thromboplastin time at 12000 ppm (both sexes). Females at 12000 ppm showed significantly lower mean values for hemoglobin concentration and red blood cell count with an associated higher mean corpuscular hemoglobin content and significantly higher mean white blood cell count and lymphocyte counts. All parameters were similar to controls at the end of the recovery period.

Significantly lower plasma proteins and globulins, and significantly higher alkaline phosphatase, alanine and asparate aminotransferase activities at 12000 ppm (both sexes). Females at 12000 ppm had higher gamma glutamyl transferase activity and higher triglyceride, cholesterol, creatinine and phosphorus levels. Males at 12000 ppm had lower mean values for cholesterol, triglycerides, glucose and higher urea values. At the end of the recovery period, the majority of these values were similar to the controls except for alkaline phosphatase activity, and in females, phosphorus values.

More samples of urine with triple phosphate crystals in males at 12000 ppm and of females with uric acid crystals at 12000 ppm. No differences existed by the end of the recovery period.

TERMINAL INVESTIGATIONS:
Treatment-related reduction of adipose tissue after 13 weeks exposure at 12000 ppm, which was not found at end of recovery period.

Statistically significant increase in mean liver weight relative to final body weight at 12000 ppm (both sexes) at the end of 13 weeks; reversible during recovery period.

Minimal to slight centrolobular hepatocytes hypertrophy and increased incidence of minimal to moderate hepatocellular pigmentation in 12000 ppm females, roughly correlating with increased liver weight. These effects were not apparent after recovery.

Test substance : Dicamba TC, Lot number 52504710, purity 89.4%, analysis date 01 November 1995

Conclusion : Oral administration of Dicamba at a dietary concentration of 12000 ppm caused a lower rate of bodyweight gain in both sexes with a reduction in food intake. This was associated with neuro-behavioral signs and significant changes in haematology and clinical chemistry parameters. Relative liver weight was increased in both sexes, probably due (at least in females) to centrolobular hepatocytes hypertrophy and to pigment deposits. Most effects were reversible after a 4-week recovery period.

No effects that could be considered to be adverse or treatment-related were seen at other dose levels.

NOAEL = 6000 ppm (479 mg/kg/day in males, 535 mg/kg/day in females)

LOAEL = 12000 ppm (1000 mg/kg/day in males, 1065 mg/kg/day in females)

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
07.12.2007 (15)

Type :
Species : rat
Sex : male/female
Strain : other: CD
Route of admin. : oral feed
Exposure period : 13 weeks
Frequency of treatm. :
Post exposure period : none
Doses : 1000, 5000 and 10000 ppm
Control group : yes
NOAEL : = 5000 ppm
Method : EPA OPP 82-1
Year : 1978
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species: Charles River CD rat
- Source: Charles River Laboratories, Portage, Michigan
- Age: exact age was not mentioned
- Weight at study initiation: male (122-164 g) female (111-145 g)
- Number of animals: 20/sex/dose group

ADMINISTRATION / EXPOSURE
- Exposure period: 13 weeks
- Route of administration: diet
- Post exposure period: none
- Doses: 1000, 5000 and 10000ppm, resulting in 69.4, 342 and 682 mg/kg bw/day for males and 79.5, 392 and 751 mg/kg bw/day for females

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: twice daily, detailed observations weekly
- Body weight: weekly
- Individueal food consumption: weekly

CLINICAL LABORATORY TESTS
In 10 rats/sex/dose group at baseline and in week 6 and 13.
- Haematology: hemoglobin, hematocrit, erythrocyte count, total and differential leukocyte counts, platelet count, mean corpuscular volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin concentrations (MCHC), and reticulocyte count.
- Biochemistry: sodium, potassium, chloride, alkaline phosphatase, blood urea nitrogen (BUN), serum glutamic pyruvate transaminase (SGPT), serum glutamic oxaloacetate transaminase (SGOT), calcium, creatinine, phosphorous, lactic dehydrogenase (LDH), glucose, total bilirubin total cholesterol, albumin, globulin, total protein.
- Urinalysis: specific gravity, volume, color and appearance, occult blood, protein, pH, bilirubin, urobilinogen, ketones, glucose, microscopic examination sediment, nitrites, urobilinogen, ketones.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: brain, heart, kidneys, liver, gonads,
- Microscopic (control animals and 10000 ppm; heart, liver, kidneys and gross lesions in all groups): all gross lesions, adrenals, eye, trachea, esophagus, stomach, duodenum, jejenum, ileum, caecum, colon, liver (2 sections), spleen, urinary bladder, testes/ ovaries, pancreas, brain (3levels-forebrain, midbrain, hindbrain), heart, lungs+mainstem bronchi, pituitary, thyroid and parathyroid, thymus, lymph node (mesenteric), sternum (bone marrow), spinal cord), salivary gland, (submaxillary), skeletal muscle (thigh), kidneys, prostate/ corpus and cervix uteri, peripheral nerve (sciatic).

ANALYSES:
- homogeneity of diet before study inititation
- stability of test article at weeks 1,3,4,8 and 13 by GC/ECD

STATISTICAL METHODS:
- analyses of variance, Bartlett and t-test as described by Steel and Torrie

Result **:** CLINICAL SIGNS/MORTALITY
- Mortality: Three female rats died during the course of the study, as follows: 1 female control (week 6), 1 female at 5000 ppm (week 2), 1 female at 10000 ppm (week 13).

- Clinical signs: No changes were seen in general behavior and appearance that were considered to be related to exposure to the test substance;
incidental findings in treated rats: rales, yellow material on the anogenital region, mouth ulcer, pale exposed skin areas, black material on or around the eye, nose, mouth or anogenital region, corneal opacity, dilated pupil, eye enlarged and protruded, increased distance between pupil and cornea, nose malaligned, swollen foot, portion of the ear missing, and portion of the tail black or missing. These signs were noted randomly among the treated rats.
One mid-dose male rat had a subcutaneous mass in the anogenital region.
Incidental findings in both treated and control rats: malaligned upper incisors, red areas around the eyes, scabbing, excessive lacrimation and hair loss.

- Body weight gain: slightly decreased at 10000 ppm in both sexes, significantly in week 13 in males.

- Food consumption: at 10000 ppm decreased consumption in both sexes.

CLINICAL CHEMISTRY
- hematology: no abnormalities; one female at 10000 ppm had elevated leucocyte, reticulocyte and platelet counts and slightly decreased hemoglobin, hematocrit and erythrocyte count
- Biochemistry: slightly elevated SAP (serum alkaline phosphatase) activity at 10000 ppm
(weeks 6 and 13) which was significant at the group means level; decreased glucose which was significant at the group means level for females at 5000 and 10000 ppm at 6 weeks and all does levels at 13 weeks and for males at 10000 ppm at 6 and 13 weeks.

- Urinalysis: no abnormalities

MACRO- AND MICROSCOPIC FINDINGS:
No gross leasion were seen.
- Organ weights: no treatment related variations
- Histopathology: absence or reduction in cytoplasmic vacuolation in hepatocytes in the high dose group (and so a reduction of liver glycogen)

ANALYSES:
- stability of test substance: after 7 day storage values ranged from 79-87% of target concentration, samples taken in week 1-4, 8 and 13 had mean concentrations of 84, 96 and 83% of target concentration for 1000, 5000 and 10000 ppm respectively.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1819-00-9 (2-methoxy-3,6-dichlorobenzoic acid), purity 86.8%

Conclusion : NOAEL 5000 ppm based on effects on body weight, food consumption and elevated ALP.

Reliability : (1) valid without restriction
20.12.2007 (16)

Type :
Species : rabbit
Sex : male/female
Strain : New Zealand white
Route of admin. : dermal
Exposure period : 3 weeks
Frequency of treatm. : 5 days a week
Post exposure period : none
Doses : 100, 500, 2500
Control group : yes
Method :
Year :
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species: New Zealand white rabbits
- Age: no data
- Weight at study initiation: males: 1.9 - 2.6 kg, females: 2.1-2.7 kg
- Number of animals: 4/sex/dose group

ADMINISTRATION / EXPOSURE
- Doses: 100, 500 and 2500 mg/kg/day
- Exposure period: 21 days
- Duration of exposure: 6 hours
- Route of administration: dermal
- Post exposure period: none
- Vehicle: 0.9% saline
- Total volume applied: no details given. Maximum vehicle amount used was 5ml.
- Area exposed: 10% of body surface
- Occlusion: not specified
- Removal of test substance: by wiping

CLINICAL OBSERVATIONS AND FREQUENCY:
- pre- and post-test determination of hematological and biochemical blood parameters (total and differential

leukocyte counts, erythrocyte count, hematocrit, hemoglobin, alkaline phosphatase, blood urea nitrogen, glutamic pyruvate transaminase, glutamic oxaloacetate transaminase, calcium, inorganic phosphorus, fasting blood glucose, albumin, total protein)
- pre- and post-test urinalysis (volume, specific gravity, color and appearance, pH, albumin, glucose, occult blood and billirubin)
- Clinical signs and mortality: daily observations, scoring of dermal irritation
- Body weight: weekly

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: The spleen, liver, adrenals, ovaries/ testes, thyroid (parathyroid), brain and kidneys were weighed fresh.
- Microscopic: skin (treated and untreated), gallbladder, lung, trachea, liver, kidneys, large intestine, small intestine, stomach, pancreas, urinary bladder, spleen, heart, regional lymph node, mesenteric lymph node, prostate/uterus, testes/ovaries, pituitary, thymus, thyroid/pars, adrenals, thyroid, eye, nerve, muscle, bone marrow, spinal cord, brain, any unusual lesions

STATISTICAL METHODS:
analysis of variance (one-way classification), Bartlett's test, Dunnett's multiple comparison tables

Result **:** TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time of death: males: 1(9) control, 1(17) 100 mg/kg; females 1(18) 100 mg/kg, 2(6&10) 500 mg/kg, 2(6&7) 2500 mg/kg

- Clinical signs:
Animals that died: diarrhea, hypoactivity, distended abdomen, anorexia and slight cyanosis.
Surviving animals diarrhea and soft stools, erythema, desquamation, atonia, coriaceousness, fissuring

- Body weight gain: no abnormalities

- Clinical chemistry: blood glucose in females at 2500 mg/kg significantly higher than controls, but within biological range

- Haematology: no abnormalities

- Urinalysis: Significant difference in pH for males at 2500 and females at 100 mg/kg compared to controls, but values were within biological range

NECROPSY FINDINGS
- Organ weights: increased adrenal weight (not toxicologically significant)

- Gross pathology:
skin thickening and erythema of the application site in 2 rabbits at 2500 mg/kg/day

- Histopathology: at application site: acanthotic epidermal thickening and hyperkeratosis, slight parakeratosis. No dose response

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 1918-00-9, (2-methoxy-3,6,-dichlorobenzoic acid), purity 86.8%
Reliability	:	(3) invalid 1. Too many animals died. From 8 control and 24 dosed rabbits one control and 6 exposed rabbits died during the study. 2. Five of the six animals that died were female rabbits. Therefore 43% of the dosed female rats did not survive the study. This was not considered in the discussion of the data. 3. The purity, stability and composition of the compound were not determined. 4. The food consumption was not monitored.

21.05.2001 (17)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA98, TA100, TA1535, TA1537 and TA102
Test concentration	:	8-5000 ug/plate
Cycotoxic concentr.	:	1500 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1983
GLP	:	yes
Test substance	:	other TS

Method :

SYSTEM OF TESTING:
- Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA102.
- Deficiences/Proficiences: histidine-requiring strains
- Metabolic activation system: rat S-9 mix, Arochlor 1254 induced

ADMINISTRATION:
- Dosing:
Mutation experiment 1 (without preincubation): 8, 40, 200, 1000, 5000µg/plate;
Mutation experiment 2: TA98, TA100, TA1535, and TA1537: 187.5, 375, 750, 1500 and 3000 ug/plate. TA102: 46.875, 93.75, 187.5, 375 and 750µg/plate.
- Number of replicates: 3
- Application: solution in DMSO
- Positive and negative control groups and treatment:
Positive controls: -S9: 2-nitrofluorene (TA98), sodium azide (TA100, TA1535), 9-aminoacridine (TA1537), gluturaldehyde (TA102).
+S9: 2-aminoanthracene (at least one strain).
Negative controls: DMSO (vehicle)
- Pre-incubation time: Mutation experiment 2; 1h incubation at 37°C of S9 with the test compound prior to addition to the tester strain.

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Dunnett's test
- Method of calculation: linear regression analysis

Result : GENOTOXIC EFFECTS:

- With metabolic activation: none
- Without metabolic activation: none
PRECIPITATION CONCENTRATION: no precipitation was observed
CYTOTOXIC CONCENTRATION: 1500 ug/plate with and without metabolic activation

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9 (3,6-dichloro-2-methoxybenzoic acid), purity 88.5%

Reliability : (1) valid without restriction

16.05.2001 (18)

Type : Chromosomal aberration test
System of testing : CHO cells
Test concentration : 300-2330 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS

Method :
- Species/cell type: Chinese hamster ovary (CHO-K1) cells
- Metabolic activation system: rat S9 mix (Aroclor 1254 induced)
- No. of metaphases analyzed: 100

ADMINISTRATION:
- Dosing: 2330, 1170, 590 and 300 µg/ml.
- Number of replicates: 2
- Application: solution in DMSO
- Exposure time: 8 hours (-S9) or 2 hours (+S9)
- Colcemid added at final concentration of 10 ug/ML
- Positive and negative control groups and treatment:
Positive controls: with S-9: triethylene melamine; without S-9: cyclophophamide
Negative controls: DMSO

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Student's t test
- method of calculation: linear regression analysis

Result : GENOTOXIC EFFECTS:
- With metabolic activation: none
- Without metabolic activation: none

PRECIPITATION CONCENTRATION: No precipitation was observed

CYTOTOXIC CONCENTRATION: No cytotoxicity was observed

STATISTICAL RESULTS: no significant increase in number of aberrations in test group compared to control group.

Positive control triethylene melamine gave 0.45 structural aberrations per cell, positive control Cyclophosphamide induced 0.69 aberrations per cell. This was in both cases a significant increase above the untreated control

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9, (3,6-dichloro-2-methoxybenzoic acid), purity 88.5%

Reliability : (2) valid with restrictions

1. Only 100 metaphases are scored (OECD 473: at least 200)

18.12.2007 (19)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Sister chromatid exchange assay
Species	:	human
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	0, 10, 50, 100, 200 and 500 ug/mL. Test substance was prepared in DMSO.
Result	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	Whole blood lymphocyte samples from three human donors were used to establish duplicate cultures at 10, 20, 50, 100, 200, and 500 ug/mL dicamba and Banvel (commercial formulation of dicamba). Dicamba was dissolved in DMSO, final solvent concentration less than 1% for all treatments. Untreated and vehicle controls were run. S9 activation was not used. Duplicate cultures were run for each donor. None of the cultures produced significant pH changes. Immediately after treatment, 0.3 ml of phytohemagluttinin M and 10 ug BrdUrd/mL were added. Cultures were then incubated for 72 hours. During the last 3 hours, cultures were treated with 0.1 ug/mL colchicine, harvested, exposed to hypotonic solution and fixed. Chromosome spreads were obtained using the air drying technique. Spreads were stained using the fluorescence-plus-Giesma staining technique. A total of 50 well-spread diploid metaphases were scored per treatment for each donor in cells which had undergone two mitoses. The data were expressed as the mean number of SCEs per cell. Kruskall-Wallis one way ANOVA was used to compare differences among donors and treatments. Two-tailed Student's t was used to compare SCE frequencies between treated and control groups. A proliferative rate index (PRI) was calculated based upon the percentage of cells which had undergone one, two or three or more mitoses. A mitotic index was also determined.
Result	:	Only the 200 ug/mL dose of dicamba induced a significant increase in SCE frequency over that in the combined controls. Cytotoxicity was observed at the highest dose, 500 ug/mL. The formulation, Banvel, induced a significant SCE frequency increase at only 500 ug/mL. Cytotoxicity was further demonstrated by an observed delay in cell-cycle progression and a significant reduction in the PRI.
Test substance	:	Dicamba, purity not reported
Reliability	:	(2) valid with restrictions

11.12.2007 (20)

Type	:	Sister chromatid exchange assay
Species	:	human
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	0, 0.1, 0.2, 0.4 and 0.8 mg/mL. Test substance was dissolved in DSMO.
Result	:	
Method	:	

Year	:	
GLP	:	
Test substance	:	other TS
Method	:	Sister chromatid exchange (SCE) assay was performed in human peripheral blood lymphocyte (HPBL) cultured in vitro. HPBL from different donors were seeded in culture plates in a volume of 5 mL RPMI 1640 medium supplemented with 2 mM glutamine and 10% human AB pooled sera. Cells were cultured at 37 degrees C in the presence of phytohemoagglutinin (1 ug/mL) and 5-bromo-2-deoxyuridine (BUDR) (10 ug/mL). Incubation with various doses (0.1 to 0.8 mg/mL) was carried out for 1.5 hr in the presence or absence of S-9 mix staring from 48 hr of culture time. Thereafter, the medium of each plate was replaced with fresh, BUDR-containing medium. Cultures were stopped at 72 hr and colcemid (0.2 ug/mL) was added during the last 2 hr. After treatment with KCl, air-dried preparations of chromosomes were performed. Differential staining of sister chromatids was done according to the fluorescence-plus-Giesma method with slight modifications. Metaphases with greater than or equal to 44 chromosomes of any of the experimental pictures were scored for SCE and results expressed as the mean SCE number of 30 metaphases.
Result	:	There was a very slight, but statistically significant increase in the number of SCEs/mitosis in dicamba-treated cultures in all three trials carried out with or without S-9 mix. Nevertheless, the SCE frequency was never double the spontaneous frequency. Therefore, a clear positive response was not achieved.
Test substance	:	Dicamba, 99% purity
Reliability	:	(2) valid with restrictions No positive control or vehicle control mentioned.

11.12.2007 (21)

Type	:	Unscheduled DNA synthesis
Species	:	other
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	0, 0.1, 0.2, 0.4 and 0.8 mg/mL
Result	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	Unscheduled DNA synthesis (UDS) was examined in human peripheral blood lymphocytes (HPBL). HPBL were obtained from two healthy adult donors and by separation on Ficoll-Hypaque density gradient. Lymphocytes (500,000 per well) were seeded in microtest plates 3040 and cultured in sextuplicate in 0.2mL of RPMI 1640 medium supplemented with 2mM glutamine and 10% human AB pooled sera. Cultures were grown at 37 deg C for 4 hours in a humidified atmosphere at 5% CO2 in the presence of 0.25 uCi/well of 3H-TdR. Pesticides were dissolved in DMSO to a final concentration in cultured cells of 1%, and their biotransformation was accomplished by adding a metabolizing system (S9 mix) to the culture. UDS was assessed by measuring 3H-TdR uptake by HPBL grown in the presence of three doses of the pesticides and 10mM hydroxyurea. At the end of culturing, lymphocytes from each culture well were harvested on glass fiber filters by a 5% trichloroacetic acid cell harvester. Radioactivity was counted in a LS-1801 Beckman liquid scintillation spectrometer. The arithmetic mean of the sextuplicate samples was calculated, and resutls are expressed as dpm +/- standard error (SE).

Result	:	Dicamba exerted dose-related toxic effects, particularly in cultures grown without S-9 mix. In cultures grown with S-9, uptake of 3H-TdR by HPBL treated at 0.4 and 0.8 mg/mL dicamba was significantly higher than that of controls. In the presence of hydroxyurea, which inhibits replicative DNS synthesis, it can be argued that the high values of 3H-TdR uptake are due to DNA repair occurring after metabolic activation of the test substance to a DNA-damaging form(s). The authors note that another study (Waters et al., 1980) did not find induction of UDS in human fetal lung fibroblasts.
Test substance	:	Dicamba, purity 99%.
Reliability	:	(3) invalid Data presented in graphical form only; no statistical analyes reported.
11.12.2007		(22)

Type	:	other
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	single dose
Doses	:	Vehicle control, positive control, 208, 416 and 832 mg/kg
Result	:	
Method	:	
Year	:	1994
GLP	:	no data
Test substance	:	other TS

Method :

Method similar to OECD Guideline for the Testing of Chemicals 475, mammalian bone marrow chromosome aberration test.

Male and female Sprague-Dawley rats aged 7-8 weeks. The range of weights was 180 +/- 20g in the experiment. All animals were housed in a controlled temperature, humidity, and lighting environment. The animals had open access to food and water. The animals were acclimatized for a period of seven days prior to the experiment.

Eight rats were used for each treatment condition (low, med, high, control). Both male and female rats were used. Dicamba was suspended in a water solution with 20% gum arabic and administered orally by gavage in a volume of 10mL/kg bw as a single dose. Negative control animals received the vehicle only.

Control and experimental animals were injected i.p. with a dose of 4 mg/kg of colcemid 1 hour prior to sacrifice. The colcemid stopped mitoses at the metaphase. 23 hours after necropsy the femurs were removed, the bone marrow removed, and the chromosomes prepared for obvservation. The classification system used in this experiment was developed by Savage (1976). A minimum of 100 metaphases was examines for aberrations for each animal.

The chi-square test was used to compare the experimental and control data ($p<0.01$).

Structural chromosome aberrations in the bone marrow of rats was investigated in this study. Three experimental groups and one control was run in this study. Each group had 4 males and 4 females. The low exposure group was treated with 208 mg/kg Dicamba, the medium 416 mg/kg, and the high 832 mg/kg (the high dose corresponds to 80% of the LD50 for Dicamba). The following chromosome aberration parameters were measured: chromosomal gaps, chromatid breaks, isochromatid breaks, fragments, and chromosomal rearrangements.

Result	:	Structural chromosome aberrations were scored for gaps, chromatid breaks, isochromatid breaks, fragments, and chromosomal rearrangements. There were no significant differences in these metrics against the vehicle control. Dicamba was non-clastogenic. No differences were seen between the two sexes.
Test substance	:	Four common pesticides with significant economic importance: cyanazine, cyhexatin, dicamba, and DNOC. Dicamba: CAS Number, 1918-00-9, purity was >/= 99%.
Reliability	:	(2) valid with restrictions
11.12.2007		(23)
Type	:	Micronucleus assay
Species	:	mouse
Sex	:	
Strain	:	ICR
Route of admin.	:	i.p.
Exposure period	:	single dose
Doses	:	450, 900 and 1800 mg/kg bw
Result	:	negative
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Species: ICR mice - Source: Harlan Sprague Dawley Inc., Frederick, MD. - Age: 6 to 8 weeks - Weight at study initiation: males (29.5 - 36.6g), females (25.5 - 32.0g) - No. of animals per dose: 15/sex/dose ADMINISTRATION: - Vehicle: deionized distilled water - Doses: 0, 450, 900, 1800 mg/kg bw. - Duration of test: Five animals of each dose group were killed after 24, 48, and 72 hr dosing. - Frequency of treatment: single dose by i.p. injection - Sampling times and number of samples: 24, 48 and 72 hours; 2-4 slides per animal - Control groups and treatment: Negative control group: vehicle 15 animals per sex. Positive control: cyclophosphamide, 5 animals per sex. EXAMINATIONS: - mortality and clinical signs - number of micronucleated Polychromatic erythrocytes (PCE)/1000 PCE - number of PCE/total erythrocyte (1000 erythrocytes scored) Evaluation of Test Results: statistical: Kastenbaum-Bowman
Remark	:	The DMA salt of dicamba is the test substance.
Result	:	Mortality: males 4/20 and 1/15, females 3/20 and 0/15 at 1800 and 900 mg/kg resp. Clinical signs: lethargy at all dose levels EFFECT ON PCE/NCE RATIO:

- number of micronucleated PCE per 1000 PCE:
450 mg/kg bw: 0.8, 0.3 and 0.2 at 24, 48 and 72 hours resp.
900 mg/kg bw: 0.9, 0.1 and 0.2 at 24, 48 and 72 hours resp.
1800 mg/kg bw: 1.4, 0.6 and 0.3 at 24, 48 and 72 hours resp.
- PCE/total erythrocytes
450 mg/kg bw: 0.65, 0.60 and 0.56 at 24, 48 and 72 hours resp.
900 mg/kg bw: 0.60, 0.58 and 0.56 at 24, 48 and 72 hours resp.
1800 mg/kg bw: 0.59, 0.52 and 0.62 at 24, 48 and 72 hours resp.

Statistical results:
micronucleated PCE/1000 PCE was not significantly increased at any dose level at any collection time in either males or females.
The positive control induced a significant increase in micronucleated PCE/1000 PCE

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : Dicamba DMA salt, purity 40.3%

Reliability : (3) invalid
1. Purity of the test substance is unknown. It is not mentioned what DMA (DMA salt of dicamba) stands for (possibly dimethylamine salt).
2. Only 1000 erythrocytes are scored for incidence of micronucleated PCE (OECD 474, 1997: at least 2000)
3. Sampling at 72 hours is too late. However 2 sampling times remain (24 and 48 hours), which is sufficient according to OECD 474, 1997.

11.12.2007 (24)

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : other: Crl:CD-(SD) BR VAF/Plus
Route of admin. : oral feed
Exposure period : Parent-generation (males/females): 10 weeks prior to mating until weaning of the litters (day 21 post-partum); F1-generation 12 weeks prior to mating until weaning of the litters (day 21 post-partum)
Frequency of treatm. : continuous
Premating exposure period
Male : 10 weeks (parental generation) or 12 weeks (F1-generation)
Female : 10 weeks (parental generation) or 12 weeks (F1-generation)
Duration of test : 50 weeks
No. of generation studies :
Doses : 500, 1500 and 5000 ppm in the diet
Control group : other: diet without the test substance
NOAEL parental : = 1500 ppm
NOAEL F1 offspring : = 1500 ppm
NOAEL F2 offspring : = 500 ppm
Method : OECD Guide-line 416 "Two-generation Reproduction Toxicity Study"
Year : 1983
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS (PARENTAL GENERATION):

- Age: males/females 6 weeks at start of treatment
- Weight at study initiation: At start of treatment males 180-271g and females 137-190g
- Source: Charles River UK Ltd
- Number of animals: 32/sex/treatment (parental), 28/sex/treatment (F1)

ADMINISTRATION / EXPOSURE
- Test duration: maximum 50 weeks
- Exposure period: males and females 10 weeks (parent generation) or 12 weeks (F1-generation) prior to mating and until weaning of the F1 or F2 generation, respectively
- Route of administration: oral via the diet
- Doses: 0, 500, 1500 and 5000 ppm in the diet

MATING PROCEDURES (PARENTAL AND F1-GENERATION):
- Mating: 1 female / 1 male (or occasionally 2 females / 1 male) during 20 days
- Day 0 of gestation: presence of vaginal plugs and/or spermatozoa in the vaginal smear of females

PARAMETERS ASSESSED DURING STUDY (PARENTAL AND F1-GENERATION):

- Mortality/clinical observations: regularly
- Body weight gain: weekly (males/females) or daily for females during mating and until parturition
- Food consumption: weekly during the premating treatment phases
- Water consumption: daily during initial and final two weeks of the premating treatment periods
- Female oestrous cycle: vaginal cytology examination 7 days prior to mating (parental generation) and the first mate of the F1-generation and during the 20-day mating period
- Male sperm analysis: at necropsy samples from both vas deferens were analysed for total count, motility and morphology (1 every 4 male rat/cage). Left testis examined for spermatid counts
- Mating and fertility data (males/females): number and days of successful matings, time between pairing and mating (with 1st or 2nd male, F1-generation)
- Maternal delivery data: duration of gestation, number pregnant, litter size (live pups) and number of implant sites
- Pup viability: number of live pups at birth and post-partum days 4, 8, 12, 16, 21 (culling on day 4 post-partum to 8 pups/litter)
- Pup observations: clinical signs, sex and external examinations; body weights on days 1 (birth), 4, 8, 12, 16 and 21 post-partum; sexual maturation of female pups by the onset of vaginal opening (as of day 28 post-partum) and of males pups by the occurrence of cleavage of the balanopreputial skinfold (as of day 35 post-partum)

ORGANS EXAMINED AT NECROPSY (PARENTAL AND F1-GENERATIONS):
- Macroscopy: all males and females (parental generation), those selected for pairing (F1-generation) and one male and one female pup from each litter (day 21 post-partum) were necropsied and gross findings recorded. The following organs were weighed: adrenals, brain, heart, kidneys, liver, lungs, pituitary, prostate (with seminal vesicles and coagulating gland) tests with

epididymides and thymus. Additionally, a full range of tissues (see microscopy) was preserved for histopathology.
Remaining pups were examined externally and internally and the sex was confirmed by gonadal inspection. Gross findings were preserved (when considered useful) for possible histopathology
- Microscopy: histopathology examinations were performed on the adrenals, aorta, bone and joint, bone marrow, brain, cranial vault, caecum, colon, duodenum, eyes, heart, ileum, jejunum, kidneys, liver, lungs, lymph nodes, mammary gland, oesophagus, ovaries, pancreas, pituitary, prostate (for F1 weanlings with seminal vesicles and coagulating gland), rectum, salivary gland, seminal vesicles (with coagulating gland) sciatic nerve, skeletal muscle, skin, spinal column, spleen, stomach, testes, epididymides, thymus, thyroids (with parathyroids), tongue, trachea (with larynx and pharynx), urinary bladder, uterus (with cervix), vagina and vas deferens

ANALYSES:
- Method: High Performance Liquid Chromatography (HPLC) with UV detection
- Sampling time: prior to start of the first premating treatment (500 ppm and 12000 ppm dietary inclusion levels) for analysis of stability and homogeneity. Samples for accuracy of exposure concentrations for each generation were taken at start of the premating treatment and at start of the mating and end of gestation/start lactation

STATISTICAL METHODS: analysis of variance, Williams' test, Kruskal-Wallis test, Analysis of covariance, Shirley's test, Fisher's exact test

Result **:** ANALYSES:
- Actual dose level: the accuracy of all test diets was acceptable (94-112% of nominal)
- Stability: stable for at least 18 days (within 91-93%)
- Homogeneity: homogeneous (all samples 91-99% of nominal)
- Actual intake during week 1-10 at 500, 1500 and 5000 ppm:
F0: males 35, 105 and 347 mg/kg bw resp., females 41, 125 and 390 mg/kg bw resp.
F1: males 40, 121 and 432 mg/kg bw resp., females 44, 35 and 458 mg/kg bw resp.

TOXIC EFFECTS BY DOSE LEVEL

PARENTAL GENERATION:

- Mortality: at 500 and 5000 ppm one female
- Body weight gain: at 5000 ppm decreased in females during pregnancy and the first week of lactation
- Food consumption/water consumption: no treatment-related findings
- Clinical signs: incidental hairless and scabbing, but no treatment-related findings
- Mating and fertility data (males/females): no differences between the dose groups (sperm motility, morphology and number normal); pregnant females at 500, 1500 and 5000 ppm: 27, 28, 29 and 27 resp.
- Maternal delivery data: at 5000 ppm slight shift of the duration of pregnancy from 22/23 to 21 days and decreased litter and pup weights
- Macroscopic examinations: pale subpleural foci on the lungs of males at 5000 ppm (parent); increased incidence of

pelvic dilations in pups (without relationship to dose)
- Organ weights:
parents: at 5000 ppm increased rel. liver weights in females, decreased epididymides, prostate and rel. kidney weight in males; at all treatments decreased pituitary weight (rel.)
pups: at 1500 ppm increased liver and decreased lung weights (both relative); at 5000 ppm decreased absolute brain weight and relative heart and lung and increased relative liver weight
- Microscopic examinations: no treatment-related findings
- Pup viability/observations: at 5000 ppm decreased pup weights and delayed sexual maturation of the males, no effects on sex ratio.

F1 GENERATION:

- Mortality: at 0, 500, 1500 and 5000 ppm, 2 males/1 female, 1 male/1 female, 1 male and 1 male, respectively
- Body weight: decreased in males at 5000 ppm and females at 5000 ppm during the first weeks after weaning
- Food consumption/water consumption: at 5000 ppm in males and females decreased (food weeks 5-8/water weeks 5-6 of premating treatment)
- Clinical signs: at 5000 ppm increased incidence of tense/stiff body tone and slow righting reflex at the latter part of lactation
- Mating and fertility data (males/females): first mate gave pregnancy rate of 56-75%; second mate 56-68%; sperm motility, morphology and number normal
- Maternal delivery data: at 5000 ppm decreased pregnancy rate (first mate), decreased litter weights; slightly higher pup loss (second mate) resulting in slightly lower litter sizes at 1500 and 5000 ppm
- Macroscopic examinations: dose related increase of the number of pale foci on the lungs in parents
- Organ weights:
parents: at 5000 ppm increased liver weights (absolute females, relative males); at all treatments kidney weight decreased relative to body weight
pups: at 5000 ppm increased relative liver weight, decreased rel. kidney and heart weight
- Microscopic examinations: no treatment-related findings
- Pup viability/observations: at 5000 ppm decreased pup weights and associated delayed male and female sexual maturation

F2 GENERATION:

- Clinical signs: no treatment-related findings
- Pup viability/observations: at 1500 slightly decreased pup weights and at 5000 ppm decreased pup weights and increased liver weights

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba technical, 3,6-dichloro-o-anisic acid), purity 86.9%

Conclusion : NO(A)EL (parents): 1500 ppm, based on decreased female body weight gain during pregnancy and increased liver weights in both sexes in the 5000 ppm group.
NO(A)EL (F1-generation): 1500 ppm, based on a marked impairment of growth of the F1-offspring and associated

reduced food and water consumption, slightly delayed sexual maturation of males and increased liver weights.
Additionally F1-females showed slightly lower body weight gain during pregnancy and signs of increased bodytone and slow righting reflex during late lactation
NO(A)EL (F2 generation): 500 ppm, based on reduced body weight gain of F1-females during pregnancy and slghtly reduced growth of F2-pups

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
10.12.2007 (25)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Crj: CD(SD)
Route of admin.	:	gavage
Exposure period	:	gestation days 6-19
Frequency of treatm.	:	Once daily
Duration of test	:	Caesarean sections on gestation day 20
Doses	:	64, 160 and 400 mg/kg/day
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 160 mg/kg bw
NOAEL teratogen.	:	= 400 mg/kg bw
NOAEL Fetotoxicity	:	= 400 mg/kg bw
Method	:	other: US 43 FR 37336, Part 163.83-3
Year	:	1981
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS
- Age: females not indicated (sexually mature)
- Weight at study initiation: 196-251g (gestation day 0)
- Number of animals: 25 (treatment/control groups)
- Source: Stone Ridge, N.Y. facilities of Charles River, Breeding Laboratories, Inc. USA

ADMINISTRATION / EXPOSURE
- Test duration: 20 days
- Exposure period: gestation days 6-19
- Route of administration: oral gavage
- Doses: 0, 64, 160 and 400 mg/kg
- Vehicle: corn oil

MATING PROCEDURES:
- Mating: 1 female / 1 male
- Day 0 of gestation: presence of copulation plug and/or sperm in the vaginal smear

PARAMETERS ASSESSED DURING STUDY:
- Mortality: twice daily
- Clinical observations: twice daily (early morning, late afternoon)
- Body weight gain: gestation days 0, 6 and 20
- Food consumption: daily (gestation days 0-19)
- Examination of uterine content: number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral

(1/3) and skeletal (2/3 foetuses) findings

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: not indicated
- Microscopy: no tissues retained

OTHER EXAMINATIONS:

No

ANALYSES:
- Method: Liquid Chromatograph (HPLC)
- Sampling time: samples taken from all preparations (1 interval subjected to analysis)

STATISTICAL METHODS: Scheffe's or Turkey's

Result **:** ANALYSES:
- Actual dose level: dose preparations were confirmed to be accurate
- Stability: Stable during at least 1 week

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

- Mortality and day of death: at 400 mg/kg 3 females died on gestation days 7 or 8
- Body weight: at 400 mg/kg decreased on gestation day 20
- Food consumption: at 400 mg/kg decreased during exposure (gestation days 6-19)
- Clinical signs: at 400 mg/kg females showed increased incidence of crusty nose/muzzle, wheezing, ataxia, stiffening of the body when held, urine soaked fur, salivation and decreased motor activity
- Number pregnant per dose level: at 0, 64, 160 and 400 mg/kg, 23, 24, 23 and 17, respectively
- Number aborting: none
- Number of resorptions (early/late): at 0, 64, 160 and 400 mg/kg, 6.4%, 3.0%, 5.3% and 8.7%, respectively (percent of implantation sites)
- Number of implantations: at 0, 64, 160 and 400 mg/kg, 14.2, 12.3, 14.3 and 13.1, respectively
- Post implantation loss: not calculated
- Number of corpora lutea: not recorded
- Duration of Pregnancy: scheduled sacrifice on gestation day 20
- Gross pathology incidence and severity: no findings

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance. Foetal body weight and sex were comparable between all groups

- Litter weights (gravid uterus): at 0, 64, 160 and 400 mg/kg, 73g, 66g, 75g and 62g, respectively
- Number viable: at 0, 64, 160 and 400 mg/kg, 13.3, 11.9, 13.6 and 11.8, respectively
- Sex ratio (percentage of males): at 0, 64, 160 and 400 mg/kg, 49.2%, 49.0%, 49.5% and 52.0%, respectively
- Body weight: at 0, 64, 160 and 400 mg/kg, for males 3.5g,

3.5g, 3.4g and 3.3g, respectively and for females 3.3g, 3.3g, 3.2g and 3.1g, respectively.
- Grossly visible abnormalities: at 160 mg/kg one foetus showed a shortened body and anurous
- Visceral abnormalities: at 400 mg/kg increased incidence renal pelvic cavitation (one litter)
- Skeletal abnormalities: at 400 mg/kg percentage incomplete frontal(s) and/or parietal(s) ossification

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba technical, 3,6-dichloro-o-anisic acid), purity 86.9%
I, CAS 1918-00-9 (technical Dicamba), purity: technical grade

Conclusion : NOAEL (maternal): 160 mg/kg based on decreased body weights and food consumption and clinical symptoms such as ataxia, stiffening of the body when held and decreased motor activity at 400 mg/kg. There were no statistically significant effects on mean number of implantation sites, resorption sites, and viable fetuses.
NOAEL (teratogenicity): 400 mg/kg based on the absence of any significantly increased malformation or variation
NOAEL (fetotoxicity): 400 mg/kg based on the absence of any effects on foetal growth or deaths

Reliability : (1) valid without restriction
No corpora lutea recorded
Post implantation loss not calculated

11.12.2007 (26)

Species : rabbit
Sex : female
Strain : New Zealand white
Route of admin. : other: oral via capsules
Exposure period : gestation days 6-18
Frequency of treatm. : Once daily
Duration of test : Caesarean sections on gestation day 29
Doses : 30, 150 and 300 mg/kg
Control group : yes, concurrent vehicle
NOAEL maternal tox. : = 30 mg/kg bw
NOAEL teratogen. : = 300 mg/kg bw
NOAEL Fetotoxicity : = 300 - mg/kg bw
Method : EPA OPP 83-3
Year : 1984
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS
- Age: females (at insemination) 26 weeks
- Weight at study initiation: 3.05-4.14 kg
- Number of animals: 20 (treatment groups), 19 (control group
- Source: Hazelton Research Products, Inc., Denver Pennsylvania, USA

ADMINISTRATION / EXPOSURE
- Test duration: 29 days
- Exposure period: gestation days 6-18
- Route of administration: oral (via capsules)
- Doses: 0, 30, 150 and 300 mg/kg
- Vehicle: opaque white gelatin capsules

MATING PROCEDURES:
- Artificial insemination: Semen collected from 4 proven

donor bucks of the same strain and source as the females. 3 hours before insemination females were intravenously injected with 20 USP units of Human Chorionic Gonadotropin. Insemination of 0.25 mL of diluted (with saline) semen sample (6.0 million spermatozoa/0.25 mL)
- Day 0 of gestation: day of insemination

PARAMETERS ASSESSED DURING STUDY:
- Mortality: twice daily
- Clinical observations: once daily or on gestation days 6-19 immediately before dosage and within 60 minutes after dosage
- Body weight gain: once weekly before insemination and on gestation days 0 and 6-29
- Food consumption: daily
- Examination of uterine content: number of corpora lutea; number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral (all foetuses) and skeletal (all foetuses) findings; brains free-hand cross-sectioned and examined for hydrocephaly

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: findings all dams recorded, all gross lesions (except commonly found parovarian cysts) were fixed for possible histopathology
- Microscopy: not performed

OTHER EXAMINATIONS:
- Uterus staining: uteri from non-pregnant rabbits were stained with 10% ammonium sulfide to comfirm absence of implantation sites

ANALYSES:
- Method: Not indicated (samples not analysed)
- Sampling time: Bulk test substance sampled on day 2 and the end of the dosing period for possible analysis

STATISTICAL METHODS: Bartlett's Test, Dunnett's Test, Kruskal-Wallis Test, Dunn's Test and Fisher's Exact Test

Result **:** ANALYSES:
- No analyses performed. Test substance dosed via capsules. Data on the identity, composition, strength, purity and stability of the test substance are kept on file with the sponsor

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

There were no differences noted among the dose groups in the number of corpora lutea, implantations, litter sizes, early and late resorptions, foetal sex ratio, foetal body weights, percent resorbed conceptuses and number of does with any resorptions

- Mortality and day of death: One female dosed at 300 mg/kg died due to an intubation error on gestation day 12. Abortion and subsequent sacrifice occurred in the 150 mg/kg dose group for 1 female on gestation day 22 and in the 300 mg/kg dose group for four females on gestation days 19 (one female), 21 (one female) and 24 (two females)

- Body weight: at 300 mg/kg body weight loss on gestation days 6-7, 6-9, 9-12, 12-15, 15-19 and overall loss during gestation days 6-19. Decreased overall body weight gain during gestation days 6-19 (loss), 6-29 and 0-29
- Food consumption: at 300 mg/kg often reduced during the dosing period resulting in a reduced overall food consumption during gestation days 6-19, 6-29 and 0-29
- Clinical signs: at 150 and 300 mg/kg females showed ataxia (and decreased motor activity). In addition, females receiving 300 mg/kg incidentally showed rales, laboured breathing, perinasal substance (red or yellow), dried faeces, impaired righting reflex, no faeces and a red substance in the cage pan
- Number pregnant per dose level: 16 (80% of number inseminated) in the 30 mg/kg group and 18 in all other groups (90-94.7% of number inseminated)
- Number aborting: at 150 mg/kg 1 and at 300 mg/kg 4
- Number of resorptions (early/late): at 0, 30, 150 and 300 mg/kg, 0.5, 0.5, 1.0 and 0.5, respectively
- Number of implantations: at 0, 30, 150 and 300 mg/kg, 6.8, 5.9, 6.4 and 6.3, respectively
- Post implantation loss: at 0, 30, 150 and 300 mg/kg, 6.4%, 4.8%, 10.1% and 7.6%, respectively
- Number of corpora lutea: at 0, 30, 150 and 300 mg/kg, 9.6, 8.4, 8.9 and 9.2, respectively
- Duration of Pregnancy: scheduled sacrifice on gestation day 29
- Gross pathology incidence and severity: no findings other then those related to intubation error (thick, hard and gray esophagus and trachea containing white mucoid substance) or commonly found parovarian cysts

There were no significant differences among the dosage groups in the litter averages for corpora lutea, implantations, litter sizes, resorptions (early and late), percent male fetuses, fetal body weights, percent resorbed conceptuses, or the number of does with any resorptions.

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance

- Litter size and weights: at 0, 30, 150 and 300 mg/kg, 6.3, 5.4, 5.4 and 5.8, respectively
- Number viable: at 0, 30, 150 and 300 mg/kg, 6.3, 5.4, 5.4 and 5.8, respectively
- Sex ratio (percentage of males): at 0, 30, 150 or 300 mg/kg, 49.4%, 64.4%, 54.7% and 54.6%, respectively
- Body weight: at 0, 30, 150 and 300 mg/kg, 44.55g, 47.11g, 44.20g and 42.47g, respectively
- Grossly visible abnormalities: incidentally observed findings consisted of umbilical hernia, menigocele, medially rotated hindlimbs, flexed hindpaws and shortened tail
- Visceral abnormalities: incidental findings comprised protrusion of the liver through the abdominal wall, agenesis of the intermediate lobe of the lungs, agenesis of the gall bladder and caudally displaced right kidney.
- Skeletal abnormalities: incidentally observed finding consisted of vertabral malformations (irregular shaped left arch of the 3rd lumbar vertebra and fosion of the left arches of the 3rd and 4th lumbar vertebrae), tail

malformation (14 vertebrae present) and variations in skull and sternal ossification (displaced nasal suture, internasal ossification site and fused 3rd and 4th sternebrae)

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : Technical dicamba, Lot No. 52625110, 90.4% active ingredient

Conclusion : NOAEL (maternal): 30 mg/kg based on the abortions, clinical signs (viz. decreased motor activity, ataxia, rales, laboured breathing, perinasal substance red/yellow, dried faeces, impaired righting reflex, no faeces, red substance in the cage pan), reduced body weight gains and reduced feed consumption
NOAEL (teratogenicity): 300 mg/kg based on the absence of any significantly increased malformation or variation
NOAEL (foetotoxicity): 300 mg/kg based on the absence of any effects on foetal growth or deaths

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

11.12.2007 (27)

(1) Sandoz Agro, Melting Point of Dicamba, Technical (1993) (89)

(2) EPI Suite, U.S. Environmental Protection Agency, 2000-2007.

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IUCLID

Data Set

Existing Chemical	:	ID: 1982-69-0
CAS No.	:	1982-69-0
Generic name	:	Benzoic acid, 3,6-dichloro-2-methoxy-sodiumsalt
Producer related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Substance related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	14.12.2007
Revision date	:	
Date of last update	:	14.12.2007
Number of pages	:	14
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 320 - 325 °C
Decomposition	:	yes, at ca. 320 - 325 °C
Sublimation	:	
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	1994
GLP	:	yes
Test substance	:	other TS
Method	:	OECD 102, capillary method was used. A metal block electrothermal melting apparatus was used. An acetanilide standard was run to ensure the proper calibration of the melting point apparatus. Two trials of the standard were run and temperatures of 114.5 and 116.5 C were recorded versus expected temperatures of 115 and 116 C. For the test substance, two simultaneous determinations were made.
Result	:	The samples in each of two capillary tubes showed no evidence of melting at any temperature below 320 degrees C. Between 320 and 325 degrees C, the samples in each tube turned dark brown in color indicating that decomposition had taken place. Liquid droplets were observed in each tube above the charred sample remains.
Test substance	:	The test substance, SAN 845 H technical, No. 30420-001 (Batch No. 6196:1) is the sodium salt of the pesticide Dicamba (sodium 2-methoxy-3,6-dichlorobenzoate), CAS number 1982-69-0. A purity of 79.4% was obtained through HPLC analysis.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

17.10.2007 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	ca. .0000000000033 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20. Experimentally determined melting point of 325 degrees C was used as a physical property input.
Result	:	Vapor Pressure Estimations (25 deg C): (Using BP: 525.94 deg C (estimated)) (Using MP: 325.00 deg C (user entered)) VP: 1.38E-014 mm Hg (Antoine Method) VP: 2.46E-012 mm Hg (Modified Grain Method) VP: 1.38E-011 mm Hg (Mackay Method) Selected VP: 2.46E-012 mm Hg (Modified Grain Method) Subcooled liquid VP: 6.02E-009 mm Hg (25 deg C, Mod-Grain method)
Test substance	:	Dicamba sodium salt, CAS 1982-69-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

17.10.2007 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -.9 at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS

Method : Estimation using KOWIN v1.67 in EPIWIN v3.20. Experimentally determined melting point of 325 degrees C was used as a physical property input.
Result :

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -0.90

SMILES : COc1c(CL)ccc(CL)c1C(=O)(O[Na])
CHEM : Dicamba sodium salt
MOL FOR: C8 H5 CL2 O3 Na1
MOL WT : 243.02

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	2	-CL [chlorine, aromatic attach]	0.6445	1.2890
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-C(=O)O [ester, aromatic attach]	-0.7121	-0.7121
Factor	1	C(=O)-O-{Na,K,Li} [coef*(1+0.5*(NUM-1))]	-3.5500	-3.5500
Const		Equation Constant		0.2290

Log Kow = -0.8992

Test substance : Dicamba sodium salt, CAS 1982-69-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.10.2007 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in :
Value : ca. 2623 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS

Method : Estimation using WSKOW v1.41 in EPIWIN 3.20. Experimentally determined melting point of 325 degrees C was used as a physical property input.

Result :

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 2623 mg/L

SMILES : COc1c(CL)ccc(CL)c1C(=O)(O[Na])
CHEM : Dicamba sodium salt
MOL FOR: C8 H5 CL2 O3 Na1
MOL WT : 243.02
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -0.90
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.90

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = 325.00 deg C (Use Tm = 25 for all liquids)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -1.967
Water Solubility at 25 deg C (mg/L): 2623

Test substance : Dicamba sodium salt, CAS 1982-69-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.10.2007 (2)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	ca. .0000000000048558 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using AOPWIN v1.92 in EPIWIN v3.20.
Result	:	AOP Program (v1.92) Results: ========== SMILES : c1(c(c(ccc1CL)CL)OC)C(=O)O([Na]) CHEM : MOL FOR: C8 H5 CL2 O3 Na1 MOL WT : 243.02 ---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.8296 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec **Addition to Aromatic Rings = 4.0262 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 4.8558 E-12 cm3/molecule-sec HALF-LIFE = 2.203 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 26.432 Hrs ..... ** Designates Estimation(s) Using ASSUMED Value(s)
Test substance	:	Dicamba sodium salt, CAS 1982-69-0
Reliability	:	(2) valid with restrictions Acceptable method of estimation.

13.12.2007 (2)

Type	:	water
Light source	:	Xenon lamp
Light spectrum	:	> 290 nm
Relative intensity	:	1.32 based on intensity of sunlight
Conc. of substance	:	100.19 mg/l at 25 °C
DIRECT PHOTOLYSIS		
Halflife t1/2	:	50.3 day(s)
Degradation	:	31.3 % after 30 day(s)
Quantum yield	:	
Method	:	A 1000 mL test solution consisting of 100.19 mg dicamba with a specific activity of 412.2 dpm/ug (total 688 kBq) in aqueous buffer solution pH 7 containing 1% acetonitrile was prepared. The test solution was incubated at 25 +/- 1 deg C under contineous stirring for 30 days. Average incident radiation on the reactor surface was 7.704E2 W/m2 (measured before and after the study). The reaction solution was aerated and connected to a silica

gel trap, an ethylene glycol trap (organic volatiles) and a 10% NaOH trap (supposed to collect CO2) in series. Before initiation of photolysis, a 50 mL sample was taken as dark control sample. 20 mL samples were taken before initiation of photolysis and on day 1, 3, 8, 15, 22 and 30.

The samples were analyzed as follows:
- duplicate 1 mL samples were analyzed by LSC
- 15 mL was extracted twice at pH < 1 with ethyl acetate, both fractions were analyzed by LSC (duplicate 1 mL samples)
- ethyl acetate fraction was dried and concentrated, and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- extracted buffer solution of day 15, 22 and 30 were lyophilized followed by acetonitrile extraction; the extract was concentrated and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- duplicate 1 mL ethylene glycol and 10% NaOH trap samples were analyzed by LSC
- silica gel traps were extracted with with methanol, which was then analyzed by LSC; residual radioactivity in the silica traps was determined by combustion
- identity of radioactivity supposed to be CO2 in 10% NaOH trap samples was confirmed for day 22 and 30 by precipitation as BaCO3 and subsequent evolution as CO2 after addition of HCl

On day 30, the reactor was washed with methanol and with acetone. Volumes were measured and 1 mL duplicatealiquots were analyzed by LSC.

Photodegradation was calculated using the SAS Regression Program.A 1000 mL test solution consisting of 100.19 mg dicamba with

Remark : The test substance for this study was dicamba (acid form) rather than the salt. In solution, at pH 7 it does not matter if the salt or acid form is used to prepare the solution.

Result : time point (days) 14C-dicamba (% of actually applied 14C-dicamba)*

0	100 (92.14% of applied 14C)
1	98.83
3	95.25
8	86.87
15	75.62
22	66.44
30	58.74 (degradation: 41.26%)
30 (dark control)	98.61

* calculated by reviewer from % of applied 14C
Unchanged dicamba was confirmed by HPLC.

All other compounds in the different fractions, separated by TLC, were <10% of applied 14C and did not match with reference standards. CO2 in the 10% NaOH trap was 11.7% of applied at day 22 and 16.6% of applied 14C at day 30. Radioactivity in the other traps was <10% of applied 14C at all time points. Reactor wash yielded 0.3% of applied activity. The mass balance was >99% and <103.5% at all time points.

Under these conditions, t1/2 of dicamba was 38.1 days; the photolysis rate constant was 0.018 day-1. Based on the spring sunlight intensity at 40 deg latitude at noon (5.83E2

W/m2) the corresponding photodegradation rate for natural sunlight will be 0.0138 day-1; t1/2 will be 50.3 days.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba), purity 99.6% by I
Conclusion : The photodegradation rate constant in spring sunlight at 40 deg latitude at noon is 0.0138 day-1; t1/2 is 50.3 days. The major photodegradation product is CO2.
Reliability : (2) valid with restrictions
1. In the calculation of t1/2, no correction for the degradation in the dark control was made. However, this will only slightly influence the results, as there was hardly any degradation in the dark control.
2. Except for sterilization of the buffer solution, no measures to guarantee sterility of the samples were described. However, as there was hardly any degradation in the dark control (which was a subsample of the sample to be irradiated), it can be assumed biodegradation was negligible.
Flag : Critical study for SIDS endpoint
13.12.2007 (3)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Degradation : = 0 - 7.6 % after 30 day(s) at pH and °C
Deg. product :
Method : other: essentially OECD 111
Year : 1981
GLP :
Test substance :

Method : Solutions of 10 ppm and 100 ppm dicamba (1.17% and 0.12% 14C-dicamba, respectively) in distilled water or aqueous buffer solutions of pH 5.0, 7.0 and 9.0 were incubated at 25 and 35 deg C for 30 days (volume 201 mL, in amber bottles in shaking water baths). Acetone concentrations were 0.5%. After 1, 7, 14, 21 and 30 days, a duplicate 1-mL sample was taken for radioassay and a duplicate 15-mL sample was taken for extraction using diethyl ether (at pH < 1). Organic and aqueous layers were first radioassayed and then analyzed using TLC and radioautography detection, followed by quantification using LSC. Samples were cochromatographed with dicamba and three metabolite reference standards.
Remark : The test substance for this study was dicamba (acid form) rather than the salt. In solution, at specific pH levels it does not matter if the salt or acid form is used to prepare the solution.
Result : There was no significant dicamba hydrolysis (i.e. equal to or less than 7.6%) at each pH value, both concentrations and both temperatures, except for 100 ppm, pH 7.0, 35 deg C at t=14, 21 and 30 days in the 100 ppm, when degradation was up to 18.5%. Total recovery was only 82.5-83.4% for these samples, whereas it was > 95 for all other samples. Radioactivity remaining in the aqueous phase after extraction was equal to or less than 1% of applied. Three unknown degradation products each constituted less than 4% of applied.
Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9 (14C-dicamba), purity not specified
Conclusion : Dicamba is stable with slight or no hydrolysis over 30 days under the conditions tested.
Reliability : (2) valid with restrictions
1. The fact that at 100 ppm, pH 7.0, 35 deg C up to 18.5% degradation occurred was disregarded because recoveries were low. However, no explanation was given for the low recoveries. It cannot be excluded that loss of radioactivity is due to hydrolysis.
2. Section "Results and discussion" contained 2 values that were not in agreement with values in tables of results.
3. No measures to guarantee sterility of the samples or to exclude oxygen from the solutions were described. However, as measured degradation percentages were very low (except at 100 ppm, pH 7.0, 35 deg C), no significant biotic degradation or oxidation can have occurred.
2. No duplicate samples at any pH.
3. pH 5.0 was tested, whereas OECD 111 prescribes pH 4.
Flag : Critical study for SIDS endpoint
13.12.2007 (4)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year :

Method : Fugacity was determined using the EQC Level III model as found in EPIWIN v3.20. Experimentally determined melting point of 325 degrees C was used as a physical property input; other input values were estimated. Equal emissions to air, water and soil were assumed.
Result : Level III Fugacity Model (Full-Output):

==========

Chem Name : Dicamba sodium salt
Molecular Wt: 243.02
Henry's LC : 3.54e-009 atm-m3/mole (Henrywin program)
Vapor Press : 2.46e-012 mm Hg (Mpbpwin program)
Liquid VP : 2.28e-009 mm Hg (super-cooled)
Melting Pt : 325 deg C (user-entered)
Log Kow : -0.9 (Kowwin program)
Soil Koc : 0.0516 (calc by model)

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	0.63	52.9	1000
Water	51.2	1.44e+3	1000
Soil	48.1	2.88e+3	1000
Sediment	0.0996	1.3e+4	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	4.71e-014	243	185	8.1	6.18
Water	1.1e-013	725	1.51e+3	24.2	50.2
Soil	3.8e-012	340	0	11.3	0

Sediment 1.07e-013 0.157 0.0586 0.00522 0.00195

Persistence Time: 980 hr
Reaction Time: 2.25e+003 hr
Advection Time: 1.74e+003 hr
Percent Reacted: 43.6
Percent Advected: 56.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 52.87
Water: 1440
Soil: 2880
Sediment: 1.296e+4
Biowin estimate: 2.191 (months)

Advection Times (hr):
Air: 100
Water: 1000

Test substance : Dicamba sodium salt, CAS 1982-69-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
13.12.2007 (2)

3.5 BIODEGRADATION

Remark : Dicamba was determined to be not readily biodgradable in a manometric respirometry test conducted according to OECD 301F [Wallace, SJ and Daniel, M , SAN 837A: Determination of the 28 day ready biodegradability. Brixham Environmental Laboratory, AstraZeneca UK Limited, Brixham, Devon TQ5 8BA, UK, Brixham Study Number AJ0222/A, 2001].

Dicamba has a half life of 31 days with a first-order rate constant of 0.0224/day in a typical midwestern agricultural soil under aerobic conditions. Dicamba is completely mineralized to CO2 under aerobic conditions with 3,6-dichlorosalicylic acid as the only major metabolite. Low levels of 2,3-dihydroxy-3,6-dichlorosalicylic acid were detected. Metabolism under anaerobic conditions is similar to that which occurred in aerobic soil except the rate of dicamba metabolism is reduced under anaerobic conditions. [Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

Based on the results of various studies, microbial degradation appears to be the important dicamba removal process in natural water. Photolysis may contribute to dicamba removal from water(Scifres CJ et al; J Environ Qual 2: 306 (1973) As cited in HSDB update of 8-09-2001.
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1982-69-0 Sodium salt of dicamba
Conclusion : Although dicamba is not readily biodegradable according to OECD 301 F, evidence exists to indicate that dicamba can biodegrade under both aerobic and anaerobic conditions. This would also be expected for the soluble salts of dicamba.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
12.12.2007

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 1000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	water
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: Charles River Breeding Laboraties, Kingston, New York
- Age: young adult
- Number: 5/sex/dose
- Weight at study initiation: 188-269 g
- Controls: no

ADMINISTRATION:
- Doses: 5000 mg/kg bw
- Doses per time period: single
- Volume administered or concentration: 50% (w/v distilled water); dose volume 10 ml/kg
- Post dose observation period: 14 days
- food withheld 24 hour pre-dosing till 1 hour after dosing

EXAMINATIONS: gross signs of systemic toxicity and mortality (at least twice daily for 14 days). Gross necropsy on visceral and thoracic cavities.

BODY WEIGHT: pre-dosing, days 0, 7 and 13

STATISTICAL METHOD: Litchfield and Wilcoxon

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: on the day of dosing: lethargy, ataxia, inactivity, salivation, limbs extended and bodies became rigid at touch or sound stimulus and slowed respiration, loose faeces and urine stains. On day 2 after dosing, all animals appeared normal.

NECROPSY FINDINGS: no significant gross pathologic findings

SEX-SPECIFIC DIFFERENCES: on day 1, all males appeared mildly lethargic, ataxic and inactive while females only appeared slightly affected.

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, 1982-69-0 (sodium salt of Dicamba), purity 20%, impurities not indicated
Conclusion	:	LD50 > 5000 mg/kg bw (= > 1000 mg a.i./kg bw)
Reliability	:	(1) valid without restriction 1. The study was conducted in compliance with GLP. However, no compliance statement was present.

13.12.2007 (5)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 400 - mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	10
Vehicle	:	physiol. saline
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: Kings Wheel Rabbitry, Mt. Vernon, Ohio - Age: young adult - Number: 5/sex/dose - Weight at study initiation: 1.65-3.05 kg - Controls: no ADMINISTRATION: - Area covered: 10% of body surface area - Occlusion: yes - Vehicle: slightly moistened with physiological saline - Doses: 2000 mg/kg bw - Removal of test substance: wiped with physiological saline EXAMINATIONS: signs of systemic toxicity and mortality (at least twice daily for 14 days). Gross necropsy on visceral and thoracic cavities. BODY WEIGHT: pre-dosing, days 0, 6 and 13 STATISTICAL METHOD: Litchfield and Wilcoxon
Result	:	MORTALITY: - Number of deaths at each dose: no deaths CLINICAL SIGNS: Moderate to slight erythema and edema (10/10), a brown cast (10/10), slight scaling (10/10), and slight atonia (1/10). BODY WEIGHTS: changes appeared normal. NECROPSY FINDINGS: no significant findings SEX-SPECIFIC DIFFERENCES: no data
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1982-69-0 (sodium salt of Dicamba), pellets, purity 20%, impurities not indicated
Conclusion	:	LD50 > 2000 mg/kg bw (= > 400 mg a.i./kg bw)
Reliability	:	(2) valid with restrictions

1. The skin was abraded, which can influence the permeability of the test substance.
2. The study was conducted in compliance with GLP. However no compliance statement was included.

13.12.2007 (6)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Widlak, A. Melting point of dicamba sodium salt, technical. Sandoz Agro, Inc. 1300 East Touhy Ave., Des Plaines, IL 60018, 1994, Laboratory ID number 480063.

(2) EPI Suite, U.S. Environmental Protection Agency, 2000-2007.

(3) Sandoz Agro, Dicamba: Photodegradation Study in pH 7 Aqueous Solution (1993) (95) unpublished study

(4) Velsicol Chemical Corporation, Hydrolysis of 14C-dicamba, 1981.

(5) Velsicol Chemical Corporation, Acute Oral Toxicity Study in Albino Rats with 20% sodium salt of Dicamba, 1982 (57).

(6) Velsicol Chemical Corporation, Acute Dermal Toxicity Study in Albino Rabbits with 20% sodium salt of Dicamba, 1982 (58).

IUCLID

Data Set

Existing Chemical	:	ID: 1984-58-3
CAS No.	:	1984-58-3
EINECS Name	:	2,5-dichloroanisole
EC No.	:	217-852-6
Molecular Formula	:	C7H6Cl2O

Producer related part

Company	:	Arcadis
Creation date	:	04.10.2007

Substance related part

Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	26.12.2007
Revision date	:	
Date of last update	:	26.12.2007
Number of pages	:	22
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 19.9 °C
Sublimation	:	
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	2004
GLP	:	yes
Test substance	:	other TS
Method	:	The melting temperature was measured according to OECD 102, using differential scanning colorimetry. A PC controlled DSC instrument (Model DSC 204 of Netzsch), calibrated with a certified set of standards, was used. Measurement was carried out with Al2O3 as a crystallization aid. A preliminary test was run between -120 and 400 degrees C. Decomposition was not observed. In the definitive test, two heating cycles were run.
Remark	:	EPIWIN v3.20 estimates the melting temperature to be 20.65 deg C.
Result	:	The melting temperature was determined to be 19.9 degrees C (mean of two heating cycles).
Test substance	:	2,5-dichloroanisole, CAS No. 1984-58-3, batch identification: release number 13418. The test substance is a liquid at room temperature.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

15.10.2007 (1)

2.2 BOILING POINT

Value	:	= 231.3 °C at 1016.1 hPa
Decomposition	:	
Method	:	OECD Guide-line 103 "Boiling Point/boiling Range"
Year	:	2004
GLP	:	yes
Test substance	:	other TS
Method	:	Determined by dynamic method according to Annex Commission Directive 92/69/EEC, A.2.
Remark	:	EPIWIN v3.20 estimates the boiling temperature to be 215.7 deg C.
Result	:	The normal boiling temperature was obtained by interpolation to be 231.0 degrees C at a vapour pressure of 1013.25.
Test substance	:	2,5-dichloroanisole, CAS No. 1984-58-3, batch identification: release number 13418. The test substance is a liquid at room temperature.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

15.10.2007 (1)

2.4 VAPOUR PRESSURE

Value	:	= .07 hPa at 25 °C
Decomposition	:	
Method	:	Directive 92/69/EEC, A.4
Year	:	2004
GLP	:	yes
Test substance	:	other TS
Method	:	The vapour pressure was determined by dynamic method according to Annex Commission Directive 92/69/EEC, A.4. Vapour pressure measurements were made over a range of 53.95 deg C - 231.30 degrees

C. The vapour pressures were extrapolated from the regression equation.

Remark : EPIWIN v3.20 estimates the vapour pressure to be 0.22 hPa (Mackay Method).

Result : The vapour pressures calculated at different temperatures are presented below:

Temp (deg C)	VP (hPa)
20	0.04
25	0.07
50	0.51

Test substance : 2,5-dichloroanisole, CAS No. 1984-58-3, batch identification: release number 13418. The test substance is a liquid at room temperature.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

09.10.2007 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water

Log pow : = 3.5 at 24 °C

pH value : = 7.4

Method : Directive 92/69/EEC, A.8

Year : 2004

GLP : yes

Test substance : other TS

Method : The experiment was performed in accordance with Annex Commission Directive 92/69/EEC, A.8, shake flask method.

Two standard solutions of the test substance were made in 50 mL of water-saturated n-octanol: 93.30 mg / 50 mL and 88.62 mg / 50 mL. Three samples were prepared from each stock solution: 1:1, 1:2, and 2:1 v/v water:octanol saturated with water at ambient temperature (= 24 +/- 1 deg C). The n-octanol phases were diluted with water / acetonitrile (45:55 v/v) following separation. The water phases were applied undiluted. Samples were analyzed for test substance content using HPLC and subsequent UV detection. For calibration, the test substance was dissolved in acetonitrile and diluted with water/acetonitrile (45:55 v/v).

Remark : EPWIN v3.20 estimates the log Pow to be 3.36.

Result : Three measurements were made for each of the two standard solutions. The resultant values for log Pow were: 3.47, 3.50, 3.45, 3.43, 3.70 and 3.62. The mean was 3.53, with a standard deviation of 0.11.

Test substance : 2,5-dichloroanisole, CAS No. 1984-58-3, batch identification: release number 13418. The test substance is a liquid at room temperature.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

15.10.2007 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

Value : = 84 - 90 mg/l at 20 °C

pH value : = 7.1 - 7.4

concentration : at °C

Temperature effects :

Examine different pol. :

pKa : at 25 °C

Description	:	
Stable	:	
Deg. product	:	
Method	:	Directive 92/69/EEC, A.6
Year	:	2004
GLP	:	yes
Test substance	:	other TS
Method	:	The experiment was performed in accordance with Annex Commission Directive 92/69/EEC, A.6, flask method. 22.14 - 30.36 mg of the TS and 50 mL of water were shaken at 30 degrees C for 24, 48, 72, and 96 hours. The mixtures were then conditioned for 24 hours at 20 degrees C and then filtered and analyzed using HPLC with UV detection. For calibration, the test substance was dissolved and diluted with water/acetonitrile.
Remark	:	EPIWIN v3.20 estimates the water solubility to be 76 mg/L at 25 deg C.
Result	:	The mean (n = 4) water solubility was 87 +/- 3 mg/L at 20 degrees C (+/- 1 degree C).
Test condition	:	The pH of the solutions was maintained at neutral (7.1-7.4).
Test substance	:	2,5-dichloroanisole, CAS No. 1984-58-3, batch identification: release number 13418. The test substance is a liquid at room temperature.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

09.10.2007 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000052463 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	
Test substance	:	

Method : Estimation using AOP program v1.92 in EPIWIN v3.20. Experimentally determined values for melting point, boiling point and water solubility were used as physical property inputs.

Result :

AOP Program (v1.92) Results:
==========
SMILES : O(c(c(ccc1CL)CL)c1)C
CHEM : Benzene, 1,4-dichloro-2-methoxy-
MOL FOR: C7 H6 CL2 O1
MOL WT : 177.03
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8296 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 4.4167 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 5.2463 E-12 cm3/molecule-sec
HALF-LIFE = 2.039 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 24.465 Hrs
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi): 1.86E-005 (Junge,Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Test substance	:	2,5-Dichloroanisole CAS 1984-58-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

15.10.2007 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C

t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	

Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichloroanisole CAS 1984-58-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	

Method	:	Fugacity was determined using the EQC Level III model as found in EPIWIN v3.20. Experimentally determined values for melting point, boiling point, and water solubility were used as physical property inputs. Equal emissions to air, soil and water were assumed.
Result	:	Level III Fugacity Model (Full-Output):

==========

Chem Name : Benzene, 1,4-dichloro-2-methoxy-
Molecular Wt: 177.03
Henry's LC : 0.00315 atm-m3/mole (Henrywin program)
Vapor Press : 0.0742 mm Hg (Mpbpwin program)
Log Kow : 3.36 (Kowwin program)
Soil Koc : 939 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	6.41	48.9	1000
Water	17.8	900	1000
Soil	74.9	1.8e+003	1000
Sediment	0.927	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	1.23e-10	1.26e+3	893	42.2	29.8
Water	2.2e-8	191	248	6.36	8.27
Soil	4.51e-8	402	0	13.4	0
Sediment	2.44e-8	1.11	0.258	0.0368	0.00861

Persistence Time: 465 hr
Reaction Time: 750 hr
Advection Time: 1.22e+003 hr
Percent Reacted: 62
Percent Advected: 38

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 48.94
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.337 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : 2,5-Dichloroanisole CAS 1984-58-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
15.10.2007 (2)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, adapted
Concentration : 50 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : < 10 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 0 day(s) = 0 %
5 day(s) < 0 %
13 day(s) < 0 %
19 day(s) < 0 %
28 day(s) < 0 %
Control substance : Aniline
Kinetic : 14 day(s) = 74 %
28 day(s) = 80 %
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year : 2004
GLP : yes
Test substance : other TS

Method : This test follows the OECD 301 F guideline for biodegradability determination through manometric respirometry.

ThOD was calculated assuming that C is mineralized to CO2, H to H2O, Na to Na2O, and the halogens to hydrogen halide. Nitrogen is elminated as ammonia and not oxidized to nitrate or nitrite; sulfur is assumed to be oxidized to a state of +VI. The resulting value was 1356 mgThOD/g test substance.

The inoculum used was municipal activated sludge from laboratory wastewater treatment plants fed with municpal sewage. The reference substance was aniline, which has a ThOD of 2393 mgThOD/g.

The exposure time was 28 days. Biodegradation was calculated as %BOD/ThOD after 28 days.

The following controls were also run: blanks, reference substance biodegradation, inhibition of the inoculum, and abiotic elimination. Seven replicates of the test substance were run. An eighth replicate, TS 8, was run so that pH determinations could be made.

Remark : OECD 301 F states under the test conditions that the pH of the experimental vessels must be maintained at pH 7.4 (+/-0.2) throughout the experiment. The results show a clear starting pH value for the aniline reference control and the blanks outside of this range; however, this was corrected by the addition of 1 drop of 1M H2SO4. This was also added to each run containing the test substance to ensure an adequate pH. pH readings were not taken during the course of the experiment. Final pH values were taken for all experimental runs and all but the reference substance and the inhibition of the inoculum control were within the accepted range.

The concentration of the test substance was reported as "about 50 mg/L." OECD 301F requires the test substance concentration to be 100 mg/L.

Test substance : The test substance is 2,5-dichloroanisole (CAS 1984-58-3), batch #13418. Purity was determined by GC analysis as 99.3%. The test substance was stored at room temperature throughout the course of the experiment.

Conclusion : The mean value of the seven test substance replicates was -10% BOD/ThOD after 28 days. Thus, the test substance falls into the <10% category and is classified as "poorly biodegradable."

Reliability : (1) valid without restriction
Substantially complies with guideline.

13.12.2007 (4)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	= 1 measured/nominal
LC0	:	= 1 measured/nominal
LC50	:	= 2.4 measured/nominal
LC100	:	= 4.7 measured/nominal
Limit test	:	no
Analytical monitoring	:	yes
Method	:	EPA OPPTS 850.1075
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method : A 96 hour semistatic test was conducted according to: EPA-Para.72-1; EPA-SEP No.540/9-85-006; OPPTS 850.1075; 92/69/EEC, Annex V, C1; and OECD 203. The rainbow trout were hatched at the testing facility and were approximately 2 months of age at the time of exposure. The mean wet weight and body length were 0.59 g and 4.2 cm respectively. The health of the animals was observed at the beginning of the experiment; no signs of sickness, injuries, or anbnormalities were observed.

The trout were acclimatized to the experimental test conditions for 14 days prior to the experiment with diet withdrawl during the last 24 hours. The test water was non-chlorinated charcoal-filtered tap water mixed with deionized water and had a harndess of approx. 100 mg/L CaCO3, a conductivity of approx. 250uS/cm (at 25 degrees C), a pH generally between 7.5-8.5, and a temperature of approx. 14-15 degrees C. During the 14 day acclimation period the dissolved oxygen content of the water was maintained above 80% of air saturation.

Dilutions of the test substance were prepared daily and separately for each vessel. The test substance was diluted in 50 L of test water to reach the following nominal concentrations (mg/L): 0, 1.0, 2.2, 5.0, 10.0, and 22.0.

The animals were assigned to a vessel according to a randomization plan prepared by the testing laboratory. The test animals were observed within 1 hour of the start of exposure and at hours 4, 24, 48, 72, and 96 for survival and toxic signs (changes in appearance, swimming behavior, comparison of behavior to the control group). Dead fish were removed from the test vessels. Temperature, oxygen content, and the pH were measured following the beginning of the exposure period, shortly before the end of each of the 4 test intervals, and hourly measurements of water temperature were made in one of the aquariums.

Test concentrations were confirmed by analysis of samples taken at 2 intervals: from freshly prepared test water and before test water renewal for the second and last interval. Samples were taken from the middle of the test vessels using a glass pipette.

The LC50 was calculated using probit analysis and 95% confidence intervals reported where possible.

Finney, D.J., Probit Analysis; Cambr. Univ. Press, 3rd ed., 1971 (certain aspects of this method have been modified).

Result : All measured concentrations were within 80-120% of nominal during the

exposure period, with mean measured concentrations 88-103% of nominal. Control animals and animals exposed to 1 mgTS/L were asymptomatic throughout the exposure period. Animals exposed to 2.2 mg/L were asymptomatic at the 1 hour interval; however, most showed apathy by the end of the exposure period and there was one mortality each at the 48 and 72 hour interaval and 2 mortalities at the 96 hour interval. Animals exposed to 5 mg/L showed apathy at 1 hour and all but 2 were dead at the 4 hour interval and all were dead at the 24 hour interval. Animals exposed to 10 mg/L and 22 mg/L were all dead at the 1 hour interval.

The effect concentrations were calculated based on the mean measured concentrations of the test substance. The LC50 at 24, 48, 72 and 96 hours was 3.2, 2.5, 2.5 and 2.4 mg/L, respectively. The NOEC at all exposure intervals was 1.0 mg/L.

Test condition : The exposure was conducted in a semistatic system with a full water renewal every 24 hours. The test vessels were glasss aquaria with a stainless steel frame (60cm x 35cm wide x 40cm high). The water depth in vessels was about 27cm. 10 animals were placed in each vessel during the experiment with 50L of test water. The loading of each vessel was 0.1 gFish/L water. Two test vessels were maintained at each experimental concentration. The light intensity was approx. 36-191 Lux and the test temperature was 14-15 deg C. The dissolved oxygen content of the test water was maintained above 60% of air saturation throughout the duration of the exposure. No aeration or feeding was conducted during the 96 hour exposure period.

Test substance : The test substance is 2,5-dichloroanisole (CAS 1984-58-3), Batch No. 13418. A certificate of analysis confirms that the purity of the substance upon testing was 99.3%. The test substance, a homogenous, colorless, liquid, was stored at room temperature.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

15.10.2007 (5)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	semistatic
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50 based on nominal concentrations	:	= 9.44
EC50 based on mean measured concentrations	:	= 5.89
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method : A semistatic test was conducted in which the test solutions were renewed after 24 hours. Daphnids aged 2-24 hours old, from in-house cultures, were used to start the test. Animals were not fed during exposure. Animals were cultured and tested in synthetic fresh water (M4 medium prepared per ISO 10706), with a hardness of 2.43 mmol/L, conductivity 602 uS/cm and pH 8.1. The M4 medium was aerated for approx. 24 hours to attain oxygen saturation.

The test substance was stirred in M4 medium for about 20 hours at 20 +/- 2

degrees C. Undissolved test substance was removed by centrifugation. The eluate appeared clear and colorless and was used to prepare six nominal test concentrations: 1.56, 3.13, 6.25, 12.5, 25 and 50 mg/L. The control was medium with no test substance added. Analytical determination of the test concentrations was performed at 0 hours, 24 hours (old and new test solutions), and 48 hours.

Four replicate test vessels (20 mL test tubes with flat glass bottoms, containing 10 mL of test solution) were used per test treatment. Five daphnids were impartially added to each test vessel (loading 0.5 animals/mL), for a total of 20 organisms per test treatment. Immobilization was observed at 0, 24, and 48 hours. Dissolved oxygen and pH were measured at 0, 24 and 48 hours in old and new test solutions. Temperature was measured continuously in a separate test vessel. The EC values were calculated using the probit method.

Result : Measured concentrations of test substance ranged from 64.9-85.9% of nominal at the beginning of the test but declined to 36.7-42.7% after 24 hours. Similar results were obtained on the fresh solutions prepared to renew the test. The mean measured concentrations ranged from 59.3%-66.7% of nominal and were: 0.925, 1.93, 3.90, 7.78, 16.0 and 33.4 mg/L.

Dissolved oxygen during the test ranged from 8.4-8.8 mg/L, pH from 8.0-8.1, and temperature from 19.7-20.1 degrees C.

By 48 hours, complete immobilization of daphnids occurred at the two highest test concentrations, with significant immobilization at 12.5 mg/L and essentially no immobilization at the lower test concentrations. No immobilization and no capture of daphnids in the surface film occurred in the controls. The resultant 48-h EC0, EC50 and EC100 values based upon the nominal concentrations were 6.25, 9.44 and 25 mg/L, respectively. The 48-h EC0, EC50 and EC100 values based upon the mean measured concentrations were 3.90, 5.89 and 16.0 mg/L, respectively.

Test condition : The test was conducted at a temperature of 18-22 degrees C (max. temperature difference 2 degrees C). Illumination was provided by warm white lights (intensity about 1-8 uE/m2s at a wavelength of 400-750 nm) on a photoperiod of 16 h day: 8 h night.

Test substance : The test substance is 2,5-dichloroanisole (CAS 1984-58-3), batch #13418. Purity was determined by GC analysis as 99.3%. The test substance was stored at room temperature throughout the course of the experiment.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

17.10.2007 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	growth rate
Exposure period	:	72 hour(s)
Unit	:	mg/l
Limit test	:	no
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method : The study was conducted according to OECD 201 and EPA OPPTS 850.5400. The test organism was Desmodesmus subspicatus (formerly known as Scenedesmus subspicatus). The nominal inoculation density used in the experiment was 1E4 cells/mL. Three replicates were run for

both the experimental vessels and the control.

The test medium was prepared according to OECD Guideline 201 (OECD medium).

The stock solutions were prepared separately for each concentration and were stirred for approx. 20 hours at 20 +/- 2 degrees C and then centriuged. The two highest test concentrations could not be centrifuged due to a technical defect of the centrifuge. For the centrifuged solutions, the supernatant was decanted and used for testing. Nominal test concentrations were 0, 3.13, 6.25, 12.5, 25 and 50 mg/L. The test substance was not completely soluble in OECD medium.

Test concentrations were run in triplicate along with a triplicate control.

The test parameter was in vivo chlorophyll-a fluorescence (435nm), which was measured in each replicate at 0, 24, 48, and 72 hour intervals by a Fluorometer EOS Fl2. Cell counting was performed after 72 hours in a counting chamber (Neubauer improved) in replicate No.2 of the inoculated control and the data used to construct a calibration curve between fluorescence and cell counts.

The temperature was continuously monitored throughout the 72 hour exposure. The pH was measured at time zero and at 72 hours in an additional uninoculated replicate and after 72 hours in the inoculated replicate No.1 of each concentration.

Result : Measured concentrations of the test substance decreased dramatically during the experiment. Analytical determinations of the test substance in the 50, 25, and 12.5 mg/L solutions showed that concentrations had decreased to 2.4-3.2% of the nominal concentrations. In the 3.13 and 6.25 mg/L solutions no test substance could be detected. The authors hypothesize that this may be due to sensitivity of the test substance to the light used in the experiment.

Population growth was completely inhibited at the highest test concentration, partially inhibited at the 25 mg/L test concentration, and unaffected at the three loweset test concentrations. Test results were calculated based upon both biomass (the integral of growth over test duration) and growth rate.

The results based on the mean analytically determined concentrations, mg/L, are:

EbC50 8.1
NOEbC 4.817

ErC50 10.1
NOErC 4.817

The results based on the nominal concentrations, in mg/L, are:

EbC50 19.2
NOEbC 12.5

ErC50 23.0
NOErC 12.5

The following test validity criteria were met: Cell multiplication in the control after 72 hours was 25-fold. Variation in pH within 72 hours in the control was not more than 2 units.

Test condition : The test vessels (250 mL Erlenmeyer flasks) were illuminated in artificial light, type white universal (ORSAM L 25), under continuous illumination.

The intensity was about 60-120 uE/(m2*s) at a wavelength of 400-700 nm.

Test substance : 2,5-dichlorophenol, Batch#13418, purity 99.3% as stated on certificate of analysis. The test substance is a homogenous, colorless, liquid.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

17.10.2007 (7)

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	males: 35 days, females: 44 days
Frequency of treatm.	:	One time per day at the same time in the morning.
Post exposure period	:	
Doses	:	0 mg/kg/d, 50 mg/kg/d, 150 mg/kg/d, 450 mg/kg/d
Control group	:	yes, concurrent vehicle
NOAEL	:	= 150 mg/kg bw
Method	:	OECD combined study TG422
Year	:	2006
GLP	:	yes
Test substance	:	other TS

Method :

Male and female Wistar rats aged 11-12 weeks were used in the study. All animals were free of disease and females non-pregnant at the beginning of the study. The males and females were raised from separate litters to prevent possible sibling mating.

Three experimental test groups, plus a control, were run with 10 animals of each sex in each group. Dosage levels were 50 mg/kg/d (the expected no adverse effect level dose), 150 mg/kg/d, and 450 mg/kg/d. The control group was treated identically to the experimental animals except for dosage of the test substance. The test substance was administered dissolved in 0.5% carboxymethylcellulose solution in double distilled water and Tween 80. Controls received 0.5% carboxymethlycellulose solution in double distilled water and Tween 80. All animals received 10 mL/kg/d of solution.

TEST SUBSTANCE PREPARATION

The test substance was weighed in a calibrated beaker, topped up with 0.5% Carboxycellulose solution in double distilled water and a few drops of Tween 80 and mixed with a magnetic stirrer. These emulsions were prepared at the beginning of the study and every 7-8 days afterward, based on the results of a stability study which indicated the test emulsions were stable at room temperature for up to 10 days. Analytical monitoring of the test substance preparations was performed at the beginning of the study.

EXPERIMENTAL PROCEDURE AND TIME SCHEDULE

Following acclimation of about 6 days, 80 animals were selected for use. The mean weight of the 40 male animals was 301.4 g (282.3-321.9) and for the 40 female animals 206.8 g (189.4-220.5). Animals were randomly assigned to test groups in a manner that resulted in similar body mass values in each experimental group.

Dosing was conducted once daily via gavage at approximately the same time each day. This was carried out until 1 day prior to sacrifice. After experimental day 13, males and females from the same dose group were placed in mating cages at a 1:1 ratio.

On study day 31 motor activity measurements and a functional observational battery were carried out on the first 5 males (by randomly assigned ID numbers) in each group. On study day 35, blood from all F0 males was sampled under Isofluorane anesthesia followed by necropsy. A functional observational battery and motor activity measurement were carried out on females on experimental day 43. Blood samples from 5 F0 females was taken under Isofluorane anesthesia on day 44 followed by necropsy.

Checks were made twice daily for moribund or dead animals (once daily on weekends and holidays). Moribund animals were necropsied. Detailed clinical observations were made in all animals once before test substance administration and at weekly intervals thereafter. Food consumption of the F0 animals was determined during premating and in dams during gestation and lactation periods. In general, body weights of F0 animals were determined once a week.

Methods relevant to the reproduction and developmental portion of this study are described in Section 5.8.1 and 5.8.2.

Result **:** FOOD CONSUMPTION: Food consumption of males in all substance-treated groups was similar to that of controls; however it was not measured during premating days 7-14. Food consumption of females in the highest dose group was significantly decreased during premating week 1 and during lactation days 0-4, and this effect was considered to be substance-related.

BODY WEIGHT / BODY WEIGHT CHANGES: Body weight for both males and females was comparable to the control group during the premating period and after weaning. The body weight changes for the high dose females were statistically significantly decreased during gestation days 0-7 and lactation days 0-4.

CLINICAL OBSERVATIONS: Temporary salivation after dosing was observed but was not assessed as an adverse or toxic effect. During study weeks 2 and 3, two out of 10 high dose males had urine smeared fur, which may be an indication of an impaired general condition. No other abnormalities were found.

FUNCTIONAL OBSERVATIONAL BATTERY: No test substance-related findings.

MOTOR ACTIVITY MEASUREMENT: No test substance-related findings.

CLINICAL PATHOLOGY: No treatment-related effects in hematology and enzymes. Slight changes observed in various blood chemistry parameters in high dose males and a marginal increase in inorganic phosphate in high dose females. These mild effects were considered to be not toxicologicaly significant and thus assessed as not being treatment-related.

PATHOLOGY: Substance-related findings occurred in the liver, thyroid glands and kidneys. The absolute and relative kidney weights of males in

the mid and top dose groups were statistically significantly increased in a dose-related manner. There was a slight increase in the incidence and severity of chronic nephropathy in the top dose group.

GROSS LESIONS: A single lesion was detected, but was unrleated to the test substance.

Test condition : Animals were housed individually in stainless steel wire mesh cages (floor area about 800 cm2), with the following exceptions: for the overnight mating, the females were put into the cages of the males; from day 18 p.c. until sacrifice, the pregnant females were housed in Makrolon cages with their litters. Cages were kept in air conditioned rooms at a temperature of 20-24 degrees C and relative humidity 30-70%. The photoperiod was 12 hours light: 12 hours dark. The food was ground Kilba maintenance diet mouse/rat, and tap water was provided for drinking water. Food and water were available ad libitum except during the fasting period and measurement of motor activity.

Test substance : 2,5-dichloroanisole, Batch# 13418, CAS# 1985-58-3. Purity 99.3% as stated on certificate of analysis.

Conclusion : The NOAEL for general, systemic toxicity of the test substance is 150 mg/kg/d for the F0 parental rats of both sexes. This is based upon impairments of food consumption and body weight data for the high dose females and a higher incidence and severity of chronic progressive nephropathy in the high dose males.

Reliability : (1) valid without restriction

26.12.2007 (8)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

Type : other: combined repeated dose with reproductive/developmental toxicity screening

Species : rat

Sex : male/female

Strain : Wistar

Route of admin. : gavage

Exposure period : males: 35 days; females: 44 days

Frequency of treatm. : once per day at the same time in the morning

Premating exposure period

Male : 13 days

Female : 13 days

Duration of test : males: 35 days; females: 44 days

No. of generation studies :

Doses : 0 mg/kg/d, 50 mg/kg/d, 150 mg/kg/d, 450 mg/kg/d

Control group : yes, concurrent vehicle

NOAEL parental : = 450 mg/kg bw

NOAEL F1 offspring : = 450 mg/kg bw

Result : NOAEL for reproductive performance and fertility is the highest dose tested, 450 mg/kg/d.

Method : OECD Guide-line 422

Year : 2006

GLP : yes

Test substance : other TS

Method : Male and female Wistar rats aged 11-12 weeks were used in the study. All animals were free of disease and females non-pregnant at the beginning of the study. The males and females were raised from separate litters to prevent possible sibling mating.

Three experimental test groups, plus a control, were run with 10 animals of each sex in each group. Dosage levels were 50 mg/kg/d (the expected no adverse effect level dose), 150 mg/kg/d, and 450 mg/kg/d. The control group was treated identically to the experimental animals except for dosage of the test substance. The test substance was administered dissolved in 0.5% carboxymethylcellulose solution in double distilled water and Tween 80. Controls received 0.5% carboxymethlycellulose solution in double distilled water and Tween 80. All animals received 10 mL/kg/d of solution.

TEST SUBSTANCE PREPARATION

The test substance was weighed in a calibrated beaker, topped up with 0.5% Carboxycellulose solution in double distilled water and a few drops of Tween 80 and mixed with a magnetic stirrer. These emulsions were prepared at the beginning of the study and every 7-8 days afterward, based on the results of a stability study which indicated the test emulsions were stable at room temperature for up to 10 days. Analytical monitoring of the test substance preparations was performed at the beginning of the study.

EXPERIMENTAL PROCEDURE AND TIME SCHEDULE

Following acclimation of about 6 days, 80 animals were selected for use. The mean weight of the 40 male animals was 301.4 g (282.3-321.9) and for the 40 female animals 206.8 g (189.4-220.5). Animals were randomly assigned to test groups in a manner that resulted in similar body mass values in each experimental group.

Dosing was conducted once daily via gavage at approximately the same time each day. This was carried out until 1 day prior to sacrifice. After experimental day 13, males and females from the same dose group were placed in mating cages at a 1:1 ratio.

Checks were made twice daily for moribund or dead animals (once daily on weekends and holidays). Moribund animals were necropsied. Detailed clinical observations were performed once prior to test substance administration and weekly thereafter. Food consumption of the F0 animals (both sexes) was determined during premating and in dams during gestation and lactation periods. In general, body weights of F0 animals were determined once a week. However, during gestation and lactation, F0 females were weighed on days 0, 7, 14, and 20 p.c., on the parturition day, and day 4 post partum. Details of motor activity measurements and functional observational battery assessments on the F0 animals are described in Section 5.4.

Males were exposed for a total of 35 days, followed by necropsy. Females were allowed to litter and rear their pups until 4 days after parturition. Females were exposed for a total of 44 days, followed by necropsy.

MATING

Males and females were mated at a 1:1 ratio for a maximum period of 2 weeks. Females were placed in the cage of the male partner overnight and then vaginal smears were performed to check for the presence of sperm. If detected, that experimental day was noted as "day 0" and the following day "day 1" post-coitum (p.c.). The mating pairs were separated upon sperm detection.

DETERMINATION OF IMPLANTATION SITES

After sacrifice the uterus and ovaries were removed and examined for implantation sites, allowing for calculation of post-implantation loss.

REPRODUCTION DATA

The pairing partners, the number of mating days until the detection of vaginal sperm, and the gestational status of the female were noted for F0 mating pairs. Mating and fertility indices were calculated for males. For females, mating, fertility, gestation and live birth indices were calculated as well post-implantation loss percentage.

Result : Results for food consumption, body weight, clinical and functional observations, motor activity, clinical pathology, gross lesions and pathology for the F0 animals are described in Section 5.4. Gross and histopathological examinations of the reproductive organs of substance-treated male and female rats did not reveal any treatment effects.

MALE REPRODUCTION DATA

The male mating index was 100% for all groups and the fertility index was between 90-100% with no clear relationship to dose.

FEMALE REPRODUCTION DATA

The female mating index was 100% for all groups. No relevant differences in the mean duration until detection of sperm were found. One female in each treated group failed to deliver pups or, upon necropsy, reveal in utero implantations, thus the fertility index was 90% for the treated groups and 100% for the control; this variation is within the normal range. One control female had implantations in utero but delivered no pups; thus the gestation index was 90% for the control. The gestation index was 100% for all treated groups. Implantation was not affected by the test substance; neither was intrauterine embryo-/fetolethality since the post-implantation losses were unaffected by treatment. The test substance did not affect the mean number of F1 pups delivered per dam nor the number of stillborn pups. The live birth index was 94-100% in all test groups. The overall conclusion is that the test substance did not adversely affect reproduction and delivery data for the F0 females.

Test condition : Animals were housed individually in stainless steel wire mesh cages (floor area about 800 cm2), with the following exceptions: for the overnight mating, the females were put into the cages of the males; from day 18 p.c. until sacrifice, the pregnant females were housed in Makrolon cages with their litters. Cages were kept in air conditioned rooms at a temperature of 20-24 degrees C and relative humidity 30-70%. The photoperiod was 12 hours light: 12 hours dark. The food was ground Kilba maintenance diet mouse/rat, and tap water was provided for drinking water. Food and water were available ad libitum except during the fasting period and measurement of motor activity.

Test substance : 2,5-dichloroanisole, Batch# 13418, CAS# 1985-58-3. Purity 99.3% as stated on certificate of analysis.

Conclusion : The NOAEL for reproductive performance and fertility was the highest dose tested, 450 mg/k/d.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

26.12.2007 (8)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	F0 parents: males: 35 days; females: 44 days
Frequency of treatm.	:	F0 animals dosed once per day at the same time in the morning
Duration of test	:	males: 35 days; females: 44 days
Doses	:	0 mg/kg/d, 50 mg/kg/d, 150 mg/kg/d, 450 mg/kg/d
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 150 mg/kg bw
NOAEL teratogen.	:	= 450 - mg/kg bw
Result	:	No test substance related signs of developmental toxicity occurred in progeny
Method	:	other: OECD 422, Combined repeated dose with reproduction/developmental toxicity screen
Year	:	2006
GLP	:	yes
Test substance	:	other TS

Method :

Male and female Wistar rats aged 11-12 weeks were used in the study. All animals were free of disease and females non-pregnant at the beginning of the study. The males and females were raised from separate litters to prevent possible sibling mating.

Three experimental test groups, plus a control, were run with 10 animals of each sex in each group. Dosage levels were 50 mg/kg/d (the expected no adverse effect level dose), 150 mg/kg/d, and 450 mg/kg/d. The control group was treated identically to the experimental animals except for dosage of the test substance. The test substance was administered dissolved in 0.5% carboxymethylcellulose solution in double distilled water and Tween 80. Controls received 0.5% carboxymethlycellulose solution in double distilled water and Tween 80. All animals received 10 mL/kg/d of solution.

TEST SUBSTANCE PREPARATION

The test substance was weighed in a calibrated beaker, topped up with 0.5% Carboxycellulose solution in double distilled water and a few drops of Tween 80 and mixed with a magnetic stirrer. These emulsions were prepared at the beginning of the study and every 7-8 days afterward, based on the results of a stability study which indicated the test emulsions were stable at room temperature for up to 10 days. Analytical monitoring of the test substance preparations was performed at the beginning of the study.

EXPERIMENTAL PROCEDURE AND TIME SCHEDULE

Following acclimation of about 6 days, 80 animals were selected for use. The mean weight of the 40 male animals was 301.4 g (282.3-321.9) and for the 40 female animals 206.8 g (189.4-220.5). Animals were randomly assigned to test groups in a manner that resulted in similar body mass values in each experimental group.

Dosing was conducted once daily via gavage at approximately the same time each day. This was carried out until 1 day prior to sacrifice. After experimental day 13, males and females from the same dose group were placed in mating cages at a 1:1 ratio.

Males and females were mated at a 1:1 ratio for a maximum period of 2 weeks. Females were placed in the cage of the male partner overnight and then vaginal smears were performed to check for the presence of sperm. If detected, that experimental day was noted as "day 0" and the following day "day 1" post-coitum (p.c.). The mating pairs were separated upon sperm

detection.

Checks were made twice daily for moribund or dead animals (once daily on weekends and holidays). Moribund animals were necropsied. Detailed clinical observations were performed once prior to test substance administration and weekly thereafter. Food consumption of the F0 animals (both sexes) was determined during premating and in dams during gestation and lactation periods. In general, body weights of F0 animals were determined once a week. However, during gestation and lactation, F0 females were weighed on days 0, 7, 14, and 20 p.c., on the parturition day, and day 4 post partum.

Males were exposed for a total of 35 days, followed by necropsy. Females were allowed to litter and rear their pups until 4 days after parturition. Females were exposed for a total of 44 days followed by necropsy.

The pups were sexed on the day of birth and weighed one day after birth. Thereafter, the body weight of pups was determined on day 4 post partum. Pups were examined daily for clinical symptoms. All pups were sacrificed on day 4 post partum and examined macroscopically for external and visceral findings at necropsy.

Details of motor activity measurements and functional observational battery assessments on the F0 animals are described in Section 5.4.

Result : Results for food consumption, body weight, clinical and functional observations, motor activity, clinical pathology, gross lesions and pathology for the F0 animals are described in Section 5.4.

The test substance did not affect the mean number of F1 pups delivered per dam nor the number of stillborn pups. The live birth index was 94-100% in all test groups. The number of cannibilized pups, however, was statistically significantly increased in one high dose dam (8 out of 15 liveborn pups); this was considered spontaneous in nature and of no relation to the test substance. The viability index was also affected by this instance of cannibalization ; however, the viability index varied between 98% and 100% in all other test and control groups. Excluding the single affected litter, the viability of the high dose group was 98%. Excluding this single litter, pup body weight and number of runts was not significantly different in the high dose group from the other treatment groups and the control.

The sex ratio of the live F1 pups on the day of birth and at 4 days post partum was unaffected by the test substance. The F1 pups did not show any clinical signs up to sacrifice. Necropsy indicated scattered findings of post mortem autolysis, empty stomach, and absent unilateral testis. These findings occurred without a clear relation to dosing and/or can be found in the historical control data at comparable or even higher incidences.

Test condition : Animals were housed individually in stainless steel wire mesh cages (floor area about 800 cm2), with the following exceptions: for the overnight mating, the females were put into the cages of the males; from day 18 p.c. until sacrifice, the pregnant females were housed in Makrolon cages with their litters. Cages were kept in air conditioned rooms at a temperature of 20-24 degrees C and relative humidity 30-70%. The photoperiod was 12 hours light: 12 hours dark. The food was ground Kilba maintenance diet mouse/rat, and tap water was provided for drinking water. Food and water were available ad libitum except during the fasting period and measurement of motor activity.

Test substance : 2,5-dichloroanisole, Batch# 13418, CAS# 1985-58-3. Purity 99.3% as stated on certificate of analysis.

Conclusion : No test substance related signs of developmental toxicity were seen in the progeny of the F0 parents up to and including the highest dose, 450 mg/kg bw/d. The number of delivered F1 pups/litter, their postnatal survival and

their body weight data remained unaffected by the test substance. Clinical and/or gross necropsy examinations of the F1 pups revealed only findings which were considered to be spontaneous in nature and not related to dose. The NOAEL for developmental toxicity in the progeny is 450 mg/kg bw/d.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
26.12.2007 (8)

(1) Physico-chemical properties of 2,5-dichloroanisole, Study No. 04/0104-1, GKS Kompetenzzentrum Analytik, BASF Aktiengesellschaft, 67056 Ludwigshafen, Deutschland, 2004.

(2) EPI Suite, U.S. Environmental Protection Agency, 2000 - 2007.

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(4) Schwarz, 2,5 Dichloroanisole: Determination of the biodegradability in the manometric respirometry test, Experimental Toxicology and Ecology
BASF Aktiengesellschaft, 67056 Ludwigshafen/Rhein, Germany, Project No: 26G0104/043161, 2004.

(5) Zok, S, 2,5-Dichloroanisole: Acute toxicity study in fish (rainbow trout) in a semistatic system over 96 hours. Experimental Toxicology and Ecology,
BASF Aktiengesellschaft, 67056 Ludwigshafen/Rhein, Germany, Project No. 12F0104/045027, 2005.

(6) Jatzek, J, 2,5-Dichloroanisole: Determination of the acute effect on the swimming ability of the water flea Daphnia magna Straus. Experimental Toxicology and Ecology,
BASF Aktiengesellschaft, 67056 Ludwigshafen/Rhein, Germany, Project No. 50E0104/043141, 2005.

(7) Werner, DI, 2,5-Dichloroanisole: Determination of the inhibitory effect on the cell multiplication of unicellular green algae. Experimental Toxicology and Ecology,
BASF Aktiengesellschaft, 67056 Ludwigshafen/Rhein, Germany, Project No. 60E0104/043145, 2005.

(8) Schneider, S, Deckardt, K, Burkhardt, S, Hellwig, J and van Ravenzwaay, B. 2,5-Dichloroanisole: combined repeated dose toxicity study with the reproduction/developmental toxicity screening test in Wistar rats oral administration by gavage, Experimental Toxicology and Ecology, BASF Aktiengesellschaft 67056 Ludwigshafen, Germany, Project No. 95R0104/04028, 2006.

IUCLID

Data Set

Existing Chemical	:	ID: 52166-72-0
CAS No.	:	52166-72-0
Generic name	:	2,5-dichlorophenol, sodium salt

Producer related part

Company	:	Arcadis
Creation date	:	05.10.2007

Substance related part

Company	:	Arcadis
Creation date	:	05.10.2007
Status	:	
Memo	:	
Printing date	:	14.12.2007
Revision date	:	
Date of last update	:	14.12.2007
Number of pages	:	14
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 350 °C
Sublimation	:	
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	2005
GLP	:	yes
Test substance	:	other TS
Method	:	OECD 102, capillary method was used. Three subsamples of the test substance were heated in a Buchi Melting Point B-540 instrument equipped with Buchi melting point capillaries. Instrument calibration was confirmed using caffeine as a reference standard and operation tested each day, prior to use, with two reference standards, benzophenone and anthraquinone. Based upon the results of a preliminary test to determine the melting point range, the test substance was heated from 340 to 375 degrees C at a rate of 1.0 degrees C per minute. The temperature at which fine droplets adhered uniformly to the wall of the melting point tube was recorded as the melting point.
Remark	:	The experimentally determined melting point agrees with the estimation made in MPBPWIN v1.42 (EPIWIN v3.20) of 350 degrees C, using the adapted Joback method.
Result	:	The melting point for each of the three subsamples was 349.8, 349.8, and 349.7 degrees C. The mean melting point was 350 degrees C.
Test substance	:	2,5-dichlorophenol, sodium salt, Batch #OTH-003030, purity 99.2%
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

15.10.2007 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	= .0000000000277 at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using MPBWIN v1.42 in EPIWIN v3.20. experimentally determined melting point of 350 degrees C was used as a physical property input.
Result	:	Vapor Pressure Estimations (25 deg C): (Using BP: 476.56 deg C (estimated)) (Using MP: 350.00 deg C (user entered)) VP: 6.72E-013 mm Hg (Antoine Method) VP: 2.08E-011 mm Hg (Modified Grain Method) VP: 1.37E-010 mm Hg (Mackay Method) Selected VP: 2.08E-011 mm Hg (Modified Grain Method) Subcooled liquid VP: 1.07E-007 mm Hg (25 deg C, Mod-Grain method)
Test substance	:	Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

15.10.2007 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	ca. .12 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using KOWWIN v1.67 in EPIWIN 3.20. Experimentally determined melting point of 350 degrees C was used as a physical property input.
Test substance	:	Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

08.10.2007 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	ca. 189.8 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using WSKOW v1.41 in EPIWIN 3.20. Experimentally determined melting point of 350 degrees C was used as a physical property input.
Result	:	Water Sol from Kow (WSKOW v1.41) Results: ========== Water Sol: 189.8 mg/L SMILES : [Na]Oc1c(CL)ccc(CL)c1 CHEM : Phenol, 2,5-dichloro-, sodium salt MOL FOR: C6 H3 CL2 O1 Na1 MOL WT : 184.99 ---------- WSKOW v1.41 Results ---------- Log Kow (estimated) : 0.12 Log Kow (experimental): not available from database Log Kow used by Water solubility estimates: 0.12 Equation Used to Make Water Sol estimate: Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction Melting Pt (Tm) = 350.00 deg C (Use Tm = 25 for all liquids)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -2.989
Water Solubility at 25 deg C (mg/L): 189.8

Test substance : Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
08.10.2007 (2)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000044167 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS

Method : Estimation using AOP Program v1.92 in EPIWIN v3.20. Experimentally determined melting point of 350 degrees C was used as a physical property input.

Result :

AOP Program (v1.92) Results:
==========
SMILES : [Na]Oc1c(CL)ccc(CL)c1
CHEM : Phenol, 2,5-dichloro-, sodium salt
MOL FOR: C6 H3 CL2 O1 Na1
MOL WT : 184.99
---- SUMMARY (AOP v1.92): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 4.4167 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 4.4167 E-12 cm3/molecule-sec
HALF-LIFE = 2.422 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 29.060 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
------- SUMMARY (AOP v1.91): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi): 0.914 (Junge,Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Test substance	:	Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

15.10.2007 (2)

3.1.2 STABILITY IN WATER

Type	:	
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C

t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	
Method	:	Fugacity was determined using the EQC Level III model as found in EPIWIN v3.20. Experimentally determined melting point of 350 degrees C was used as a physical property input; other input values were estimated. Equal emissions to air, soil and water were assumed.
Result	:	Level III Fugacity Model (Full-Output):

==========

Chem Name : Phenol, 2,5-dichloro-, sodium salt
Molecular Wt: 184.99
Henry's LC : 5.49e-007 atm-m3/mole (Henrywin program)
Vapor Press : 2.08e-011 mm Hg (Mpbpwin program)
Liquid VP : 3.41e-008 mm Hg (super-cooled)
Melting Pt : 350 deg C (user-entered)
Log Kow : 0.12 (Kowwin program)
Soil Koc : 0.54 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.983	58.1	1000
Water	48.2	900	1000
Soil	50.8	1.8e+003	1000
Sediment	0.0936	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.12e-012	278	233	9.27	7.78
Water	1.7e-011	881	1.14e+003	29.4	38.1

Soil 6.35e-010 464 0 15.5 0

Sediment 1.63e-011 0.19 0.0445 0.00634 0.00148

Persistence Time: 791 hr
Reaction Time: 1.46e+003 hr
Advection Time: 1.72e+003 hr
Percent Reacted: 54.1
Percent Advected: 45.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 58.13
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.377 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
15.10.2007 (2)

3.5 BIODEGRADATION

Deg. product :
Method : other: estimated
Year :
GLP :
Test substance : other TS

Method : Estimation using BIOWIN v4.10 in EPIWIN v3.20. Experimentally determined melting point of 350 degrees C was used as a physical property input. All other parameters were the default values found in EPIWIN.

Result : BIOWIN v4.10 predicts that the test substance is not readily degradable with primary biodegradation occurring in days - weeks and ultimate biodegradation occurring in weeks - months.

BIOWIN (v4.10) Program Results:
==========
SMILES : [Na]Oc1c(CL)ccc(CL)c1
CHEM : Phenol, 2,5-dichloro-, sodium salt
MOL FOR: C6 H3 CL2 O1 Na1
MOL WT : 184.99
---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

Test substance : Phenol, 2,5-dichloro-, sodium salt. CAS 52166-72-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
14.12.2007 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	= 1.3 measured/nominal
LC50	:	= 3.2 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method :

A 96-hour flow-through test was conducted according to OECD Guideline 203 and U.S. EPA OPPTS 850.1075. Juvenile rainbow trout were held under test conditions for at least 14 days prior to the test and not fed for at least 2 days prior to the test or during the test. The mean total length of the test fish was 5.1 cm (range 4.7-5.3 cm) and the mean wet weight was 1.0 g (range 0.69-1.1 g). The dilution water was well water with specific conductance 270 umhos/cm, hardness 136 mg/L CaCO3, and alkalinity 176 mg/L CaCO3.

A primary stock solution of the test substance was prepared in N,N-dimethylformamide (DMF). Secondary stock solutions were also prepared in DMF. Aliquots of the appropriate stock solution were injected into mixing chambers of a continuous-flow diluter to attain five test concentrations (0.63, 1.3, 2.5, 5.0 and 10 mg a.i./L, nominal) as well as a negative control and solvent control. The concentration of DMF in all test treatments and solvent control was 0.1 mL/L. All test solutions appeared clear and colorless. Delivery of test substance was initiated 5 days prior to introduction of the fish. Two replicate test chambers (25 L Teflon-lined stainless steel aquaria containing approx. 15 L test water) were used for each concentration and control, with 10 fish in each. Approx. 10 volume additions of water were received by each test chamber every 24 hours.

Analytical confirmation of test concentrations was performed prior to test initiation and at 0, 48 and 96 hours. Analyses were performed by HPLC using a validated analytical method.

Observations were made at 7, 24, 48 and 72 hours after test initiation to record mortality and any abnormal behavior. Temperature, dissolved oxygen and pH were also recorded at 24-hour intervals in at least one replicate test chamber.

Result :

Measured concentrations ranged from 99-106% of nominal during the exposure period. Test results were based upon mean measured concentrations which were: 0.66, 1.3, 2.6, 5.0, and 10 mg a.i./L. All fish exposed to the two highest test concentrations died, with signs of toxicity evident among the surviving fish at 2.6 mg a.i./L. The NOEC was 1.3 mg a.i./L. The 96-hour LC50, calculated using binomial probability with non-linear interpolation, was 3.2 mg a.i./L (95% confidence interval: 2.6-5.0 mg a.i./L).

Test condition :

Test chambers were kept in a water bath at 12 +/- 1 degrees C. A photoperiod of 16 hours light and 8 hours dark (with a 30 minute transition period) was used. Dissolved oxygen was maintained at greater than 7.9 mg/L (73% saturation). The pH during the test was 8.3 - 8.4.

Test substance	:	2,5-dichlorophenol, sodium salt, Batch #OTH-003030, purity 99.2%
Reliability	:	(1) valid without restriction

15.10.2007 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	= 5.8 measured/nominal
EC50	:	= 15 measured/nominal
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method :

A 48-hour static acute toxicity test was conducted according to OECD Guideline 202 and U.S. EPA OPPTS 850.1010. Daphnid neonates (less than 24 hours old) used in the test were obtained from adults maintained in laboratory cultures in water from the same source and at approx. the same temperature as used in the test. Test organisms were not fed during the test. The dilution water was well water with specific conductance 320 umhos/cm, hardness 128 mg/L CaCO3, alkalinity 182 mg/L CaCO3, and TOC less than 1 mg/L.

A primary stock solution of the test substance was prepared in dilution water and used to prepare five nominal test concentrations: 0.78, 1.6, 3.1, 6.3 and 13 mg a.i./L. The control was dilution water. All test solutions appeared clear and colorless. There were two replicate test chambers (250 mL glass beakers) with 10 daphnids in each, for a total of 20 organisms per test treatment.

Analytical confirmation of the test concentrations was performed at test initiation and termination. Analyses were performed by HPLC using a validated analytical method.

Observations were made approx. 20, 24 and 48 hours after test initiation to record the number of dead and immobile organisms and any abnormal behavior. Temperature, dissolved oxygen and pH were recorded in each test chamber at 24 hour intervals.

Result : Measured concentrations ranged from 87-97% of nominal during the exposure period. Test results were based on mean measured concentrations which were: 0.70, 1.4, 2.9, 5.8, 12 and 24 mg a.i./L. Daphnids in the negative control and four lowest test concentrations appeared normal throughout the test, with no mortalities or immobile organisms. Complete mortality was observed at 24 mg a.i./L. The NOEC was 15 mg a.i./L. The 48-hour EC50, determined by binomial probability with non-linear interpolation, was 15 mg a.i./L (95% confidence interval: 12 - 24 mg a.i./L).

Test condition : Test vessels were kept in an environmental chamber at 20 +/- 1 degrees C. A photoperiod of 16 hours light and 8 hours dark (with a 30 minute transition period) was used. Dissolved oxygen was maintained at greater than 8.3 mg/L (92% of saturation). The pH during the test was 8.3 to 8.6.

Test substance : 2,5-dichlorophenol, sodium salt, Batch #OTH-003030, purity 99.2%

Reliability : (1) valid without restriction

15.10.2007 (5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: biomass, growth rate and area under the curve
Exposure period	:	96 hour(s)
Unit	:	mg/l
ErC50	:	= .78 measured/nominal
EyC50	:	= .34 - measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2005
GLP	:	yes
Test substance	:	other TS

Method :

The study was conducted according to OECD Guideline 201, EU Directive 92/69/EEC Method C.3, and U.S. EPA OPPTS 850.5400. The exposure period was 96 hours. Endpoints (EC50 and NOEC) were determined based upon cell density (yield), area under the growth curve, and growth rate, and were calculated at 72 hours and 96 hours. Algae were cultured and tested in freshwater algal medium, pH 7.6, prepared according to ASTM E1218-90e. Test vessels were 250 mL Erlenmeyer flasks, with three replicates per treatment. A primary stock solution of the test substance was prepared in algal medium; a secondary stock solution was used to prepare nominal test concentrations of 0.031, 0.063, 0.13, 0.25, 0.5 and 1.0 mg active ingredient (a.i.) per mL. All test solutions appeared clear and colorless. The control contained algal medium. Test vessels were inoculated with 10,000 cells/mL. At 24-hour intervals, samples were collected and refrigerated prior to enumeration. Cell counts were made using an electronic particle counter. Microscopic examination for atypcial cell morphology was performed at test termination. Concentrations of test substance were measured at 0 and 96 hours by HPLC using a validated analytical method. At 96 hours, a recovery phase was initiated to determine if algal populations exposed to 1.0 mg/L were able to grow when resuspended into fresh medium.

Result :

Measured concentrations ranged from 95-101% of nominal at test initiation but <LOQ to 30% at 96 hours. Test results were calculated based upon initial measured concentrations. Cell density in the controls increased by more than a factor of 16 within 72 hours, indicating test acceptability. Growth was maximally inhibited at the highest test concentration (1.0 mg/L), but exposed cells recovered when transferred to clean algal medium, indicating the test substance was algistatic but not algicidal.

At 72 hours, the test endpoints (with 95% confidence interval) were (expressed as mg a.i./L):
EyC50 (based upon cell density or yield): 0.31 (0.27-0.35);
ErC50 (based upon growth rate): 0.70 (0.67-0.75);
NOEC, yield: 0.12
NOEC, growth rate: 0.12

At 96 hours, the test endpoints (with 95% confidence interval) were (expressed as mg a.i./L):
EyC50 (based upon cell density or yield): 0.34 (0.31-0.38);
ErC50 (based upon growth rate): 0.78 (0.75-0.82);
NOEC, yield: 0.12
NOEC, growth rate: 0.25

Test condition :

Test vessels were held in an environmental chamber at 24 +/- 2 degrees C. and continuous cool-white fluorescent lighting of 4300 +/- 10% lux. Test vessels were continuously shaken at 100 rpm. The pH of each treatment and control was measured at test initiation and termination.

Test substance : 2,5-dichlorophenol, sodium salt, Batch #OTH-003030, purity 99.2%

Reliability : (1) valid without restriction
15.10.2007 (6)

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Lezotte, FJ and Nixon, WO. Determination of the melting point/melting range of 2,5-Dichlorophenol (sodium salt), Wildlife International, Ltd., 8598 Commerce Drive, Easton, MD, Study No. 147C-127, 2005.

(2) EPI Suite, U.S. Environmental Protection Agency, 2000-2007.

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(4) Palmer SJ, Kendall TZ, and Krueger HO. 2,5-Dichlorophenol (sodium salt): A 96-hour flow-through acute toxicity test with the rainbow trout (Oncorhynchus mykiss), Wildlife International, Ltd., 8598 Commerce Drive, Easton, MD, Study No. 147A-203, 2005.

(5) Palmer SJ, Kendall TZ, and Krueger HO. 2,5-Dichlorophenol (sodium salt): A 48-hour static acute toxicity test with the cladoceran (Daphnia magna), Wildlife International, Ltd., 8598 Commerce Drive, Easton, MD, Study No. 147A-202, 2005.

(6) Desjardins D, Kendall TZ and Krueger, HO. 2,5-Dichlorophenol (Sodium Salt): A 96-hour toxicity test with the freshwater alga (Selenastrum capricornutum), Wildlife International Ltd., 8598 Commerce Drive, Easton, MD 21601, Study No. 147A-204, 2005.

IUCLID

Data Set

Existing Chemical	:	ID: 68938-79-4
Memo	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium potassium salt
CAS No.	:	68938-79-4
Generic name	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium potassium salt

Producer related part

Company	:	Arcadis
Creation date	:	04.10.2007

Substance related part

Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	14.12.2007
Revision date	:	
Date of last update	:	14.12.2007
Number of pages	:	10
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 220 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20.
Result	:	MPBPWIN (v1.42) Program Results: ========== Experimental Database Structure Match: no data SMILES : O([Na])C(=O)c1c(O(K))c(CL)ccc1CL CHEM : MOL FOR: C7 H2 CL2 O3 Na1 K1 MOL WT : 267.09 ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 515.41 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 187.28 deg C (Gold and Ogle Method) Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods) Selected MP: 219.80 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

14.12.2007 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .000001 at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20.
Result	:	MPBPWIN (v1.42) Program Results: ========== Experimental Database Structure Match: no data SMILES : O([Na])C(=O)c1c(O(K))c(CL)ccc1CL CHEM : MOL FOR: C7 H2 CL2 O3 Na1 K1 MOL WT : 267.09 ---------- SUMMARY MPBPWIN v1.42 ----------

Boiling Point: 515.41 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 187.28 deg C (Gold and Ogle Method)
Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods)
Selected MP: 219.80 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 515.41 deg C (estimated))
(Using MP: 219.80 deg C (estimated))
VP: 7.85E-013 mm Hg (Antoine Method)
VP: 9.27E-011 mm Hg (Modified Grain Method)
VP: 2.81E-010 mm Hg (Mackay Method)
Selected VP: 9.27E-011 mm Hg (Modified Grain Method)
Subcooled liquid VP: 1.12E-008 mm Hg (25 deg C, Mod-Grain method)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. -4.15 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Method : Estimation using KOWWIN v1.67 in EPIWIN v3.20.
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
14.12.2007 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in :
Value : ca. 1000 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated from Ko/w estimate
Year :
GLP : no

Test substance : other TS

Method : Estimation using WSKOW v1.41 in EPIWIN v3.20.
Result : Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 1e+006 mg/L

SMILES : O([Na])C(=O)c1c(O(K))c(CL)ccc1CL
CHEM :
MOL FOR: C7 H2 CL2 O3 Na1 K1
MOL WT : 267.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -4.15
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -4.15

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : 2.393
Log Water Solubility (in moles/L) : 0.573 (Applied Upper Limit)
Water Solubility at 25 deg C (mg/L): 1e+006

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
14.12.2007 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000
Rate constant	:	ca. .0000000000040262 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using APOWIN v1.90 in EPIWIN v3.20.
Result	:	AOP Program (v1.92) Results: ========== SMILES : O([Na])C(=O)c1c(O(K))c(CL)ccc1CL CHEM : MOL FOR: C7 H2 CL2 O3 Na1 K1 MOL WT : 267.09 --------- SUMMARY (AOP v1.92): HYDROXYL RADICALS --------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec **Addition to Aromatic Rings = 4.0262 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 4.0262 E-12 cm3/molecule-sec HALF-LIFE = 2.657 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 31.879 Hrs ** Designates Estimation(s) Using ASSUMED Value(s) --------- SUMMARY (AOP v1.91): OZONE REACTION ---------- ****** NO OZONE REACTION ESTIMATION ****** (ONLY Olefins and Acetylenes are Estimated) Experimental Database: NO Structure Matches Fraction sorbed to airborne particulates (phi): 0.99 (Junge,Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4.
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

14.12.2007 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C

t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other: estimated
Year	:	2001
GLP	:	
Test substance	:	

Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9. The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	
Year	:	

Method	:	Fugacity was determined using EQC Level III model as found in EPIWIN v3.20. Equal emissions to air, soil, and water were assumed. Parameters used were the default values found in EPIWIN.
Result	:	Level III Fugacity Model (Full-Output): ========== Chem Name : Molecular Wt: 267.09 Henry's LC : 3.26e-017 atm-m3/mole (calc VP/Wsol) Vapor Press : 9.27e-011 mm Hg (Mpbpwin program) Liquid VP : 7.83e-009 mm Hg (super-cooled) Melting Pt : 220 deg C (Mpbpwin program) Log Kow : -4.15 (Kowwin program) Soil Koc : 2.9e-005 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.41e-008	63.8	1000
Water	49.5	1.44e+003	1000
Soil	50.4	2.88e+003	1000
Sediment	0.0962	1.3e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	1.22e-20	1.68e-5	1.55e-5	5.6e-7	5.15e-7

Water	1.06e-21	836	1.74e+3	27.9	57.9
Soil	4e-20	426	0	14.2	0
Sediment	1.03e-21	0.181	0.0675	0.00602	0.00225

Persistence Time: 1.17e+3 hr
Reaction Time: 2.78e+3 hr
Advection Time: 2.02e+3 hr
Percent Reacted: 42.1
Percent Advected: 57.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 63.77
Water: 1440
Soil: 2880
Sediment: 1.296e+4
Biowin estimate: 2.196 (months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
14.12.2007 (1)

3.5 BIODEGRADATION

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Conclusion : Although dicamba is readily biodegradable according to OECD 301 F, evidence exists to indicate that dicamba can biodegrade under both aerobic and anaerobic conditions. This would also be expected for the soluble salts of dicamba.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
13.12.2007 (3)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	ca. 1562 - mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	
Remark	:	This value comes from the literature for 2-hydroxy-3,6-dichlorobenzoic acid which is expected to have similar acute toxicity as its soluble salts.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid CAS 3401-80-7.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPI Suite, U.S. Environmental Protection Agency, 2000-2007.

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(3) Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

(4) Pis'ko, GT, Tolstopjatova, GV, and AI Tovstenko AI Comparative study of the toxicity of 2-hydroxy-3,6-dichlorobenzoic acid by various routes of administration Gigiena truda i professional'nye zabolevanija Sep. 1981, No.9, p.55-56.

IUCLID

Data Set

Existing Chemical	:	ID: 68938-80-7
CAS No.	:	68938-80-7
Generic name	:	3,6-dichloro-2-hydroxybenzoic acid, dipotassium salt
Producer related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Substance related part		
Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	14.12.2007
Revision date	:	
Date of last update	:	14.12.2007
Number of pages	:	10
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 220 °C
Sublimation	:	
Method	:	other: estimated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20.
Result	:	MPBPWIN (v1.42) Program Results: ========== Experimental Database Structure Match: no data SMILES : O(K)C(=O)c1c(O(K))c(CL)ccc1CL CHEM : MOL FOR: C7 H2 CL2 O3 K2 MOL WT : 283.19 ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 515.41 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 187.28 deg C (Gold and Ogle Method) Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods) Selected MP: 219.80 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

25.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .0001 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20.
Result	:	MPBPWIN (v1.42) Program Results: ========== Experimental Database Structure Match: no data SMILES : O(K)C(=O)c1c(O(K))c(CL)ccc1CL CHEM : MOL FOR: C7 H2 CL2 O3 K2 MOL WT : 283.19 ---------- SUMMARY MPBPWIN v1.42 ----------

Boiling Point: 515.41 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 187.28 deg C (Gold and Ogle Method)
Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods)
Selected MP: 219.80 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 515.41 deg C (estimated))
(Using MP: 219.80 deg C (estimated))
VP: 7.85E-013 mm Hg (Antoine Method)
VP: 9.27E-011 mm Hg (Modified Grain Method)
VP: 2.81E-010 mm Hg (Mackay Method)
Selected VP: 9.27E-011 mm Hg (Modified Grain Method)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
25.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. -4.15 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Method : Estimation using KOWWIN v1.67 in EPIWIN v3.20.
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
13.12.2007 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in :
Value : ca. 100000 at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: estimated
Year :
GLP : no
Test substance : other TS

Method : Estimation using WSKOW v1.41 in EPIWIN v3.20.

Result : Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 1e+006 mg/L

SMILES : O(K)C(=O)c1c(O(K))c(CL)ccc1CL
CHEM :
MOL FOR: C7 H2 CL2 O3 K2
MOL WT : 283.19
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -4.15
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -4.15

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : 2.275
Log Water Solubility (in moles/L) : 0.548 (Applied Upper Limit)
Water Solubility at 25 deg C (mg/L): 1e+006

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
13.12.2007 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	ca. .0000000000040262 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS

Method : Estimation using APOWIN v1.92 in EPIWIN v3.20.

Result :

```
AOP Program (v1.92) Results:
==========================
SMILES : O(K)C(=O)c1c(O(K))c(CL)ccc1CL
CHEM   :
MOL FOR: C7 H2 CL2 O3 K2
MOL WT : 283.19
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ----------
Hydrogen Abstraction      =   0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings =   4.0262 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

  OVERALL OH Rate Constant =   4.0262 E-12 cm3/molecule-sec
  HALF-LIFE =     2.657 Days (12-hr day; 1.5E6 OH/cm3)
  HALF-LIFE =    31.879 Hrs
..........  ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------

          ******  NO OZONE REACTION ESTIMATION ******
          (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches
Fraction sorbed to airborne particulates (phi): 0.99 (Junge,Mackay)
   Note: the sorbed fraction may be resistant to atmospheric oxidation
```

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C

t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other: estimated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9. The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: estimated
Year	:	
Method	:	Fugacity was determined using EQC Level III model as found in EPIWIN v3.20. Equal emissions to air, water, and soil were assumed. Parameters used were the default values found in EPIWIN.
Result	:	Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 283.19
Henry's LC : 3.45e-017 atm-m3/mole (calc VP/Wsol)
Vapor Press : 9.27e-011 mm Hg (Mpbpwin program)
Liquid VP : 7.83e-009 mm Hg (super-cooled)
Melting Pt : 220 deg C (Mpbpwin program)
Log Kow : -4.15 (Kowwin program)
Soil Koc : 2.9e-005 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.67e-008	63.8	1000
Water	49.5	1.44e+003	1000
Soil	50.4	2.88e+003	1000
Sediment	0.0962	1.3e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	1.22e-20	1.78e-5	1.64e-5	5.94e-7	5.47e-7
Water	1.06e-21	836	1.74e+3	27.9	57.9

Soil	4e-20	426	0	14.2	0
Sediment	1.03e-21	0.181	0.0675	0.00602	0.00225

Persistence Time: 1.17e+003 hr
Reaction Time: 2.78e+003 hr
Advection Time: 2.02e+003 hr
Percent Reacted: 42.1
Percent Advected: 57.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 63.77
Water: 1440
Soil: 2880
Sediment: 1.296e+004
Biowin estimate: 2.160 (months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
13.12.2007 (1)

3.5 BIODEGRADATION

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Conclusion : Although dicamba is readily biodegradable according to OECD 301 F, evidence exists to indicate that dicamba can biodegrade under both aerobic and aerobic conditions. This would also be expected for the soluble salts of dicamba.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
14.12.2007 (3)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	ca. 1562 - ml/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	
Remark	:	This value comes from the literature for 2-hydroxy-3,6-dichlorobenzoic acid which is expected to have similar acute toxicity as its soluble salts.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid. CAS 3401-80-7
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPI Suite, U.S. Environmental Protection Agency, 2000-2007.

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(3) Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

(4) Pis'ko, GT, Tolstopjatova, GV, and AI Tovstenko AI Comparative study of the toxicity of 2-hydroxy-3,6-dichlorobenzoic acid by various routes of administration Gigiena truda i professional'nye zabolevanija Sep. 1981, No.9, p.55-56.

IUCLID

Data Set

Existing Chemical	:	ID: 68938-81-8
CAS No.	:	68938-81-8
Generic name	:	2,5-dichlorophenol, potassium salt

Producer related part

Company	:	Arcadis
Creation date	:	04.10.2007

Substance related part

Company	:	Arcadis
Creation date	:	04.10.2007
Status	:	
Memo	:	
Printing date	:	14.12.2007
Revision date	:	
Date of last update	:	14.12.2007
Number of pages	:	15
Chapter (profile)	:	Chapter: 1.0.1, 1.2, 1.6.1, 1.6.2, 1.8.1, 1.8.3, 1.8.4, 1.8.5, 1.10, 1.11, 2, 3, 4, 5, 7
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.2 SYNONYMS AND TRADENAMES

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

2.1 MELTING POINT

Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20.
Remark	:	Value of 350 deg C from Adapted Joback Method agrees with experimentally derived melting point for 2,5-dichlorophenol sodium salt.
Result	:	MPBPWIN (v1.42) Program Results: ========== Experimental Database Structure Match: no data SMILES : KOc1c(CL)ccc(CL)c1 CHEM : Phenol, 2,5-dichloro-, potassium salt MOL FOR: C6 H3 CL2 O1 K1 MOL WT : 201.09 ---------- SUMMARY MPBPWIN v1.42 ---------- Boiling Point: 476.56 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 164.60 deg C (Gold and Ogle Method) Mean Melt Pt : 257.22 deg C (Joback; Gold,Ogle Methods) Selected MP: 201.65 deg C (Weighted Value)
Test substance	:	Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	ca. .00000000195 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using MPBPWIN v1.42 in EPIWIN v3.20. Experimentally determined melting point value of 350 deg C was used for 2,5-dichlorophenol sodium salt. All other parameters used were the default values found in EPIWIN.

Result	:	MPBPWIN (v1.42) Program Results: ========== Vapor Pressure Estimations (25 deg C): (Using BP: 476.56 deg C (estimated)) (Using MP: 201.65 deg C (estimated)) VP: 4.71E-011 mm Hg (Antoine Method) VP: 1.46E-009 mm Hg (Modified Grain Method) VP: 4.04E-009 mm Hg (Mackay Method) Selected VP: 1.46E-009 mm Hg (Modified Grain Method) Subcooled liquid VP: 1.07E-007 mm Hg (25 deg C, Mod-Grain method)
Test substance	:	Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	ca. .12 at °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using KOWWIN v1.67 in EPIWIN v3.20. Experimentally determined melting point value of 350 deg C for 2,5-dichlorophenol sodium salt was used. All other parameters used were the default values found in EPIWIN.
Test substance	:	Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

13.12.2007 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	ca. 183.6 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using WSKOW v1.41 in EPIWIN v3.20. Experimentally determined melting point value of 350 deg C for 2,5-dichlorophenol sodium salt was used. All other parameters used were the default values found in EPIWIN.

Result : Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 183.6 mg/L

SMILES : O(K)c1c(CL)ccc(CL)c1
CHEM :
MOL FOR: C6 H3 CL2 O1 K1
MOL WT : 201.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 0.12
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 0.12

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = 350.00 deg C (Use Tm = 25 for all liquids)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -3.039
Water Solubility at 25 deg C (mg/L): 183.6

Test substance : Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
13.12.2007 (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	ca. .0000000000044167 cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	Estimation using APOWIN v1.92 in EPIWIN v3.20. Experimentally determined melting point value of 350 deg C for 2,5-dichlorophenol sodium salt was used. All other parameters used were the default values found in EPIWIN.
Result	:	AOP Program (v1.92) Results: ========== SMILES : O(K)c1c(CL)ccc(CL)c1 CHEM : MOL FOR: C6 H3 CL2 O1 K1 MOL WT : 201.09 ---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec **Addition to Aromatic Rings = 4.4167 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 4.4167 E-12 cm3/molecule-sec HALF-LIFE = 2.422 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 29.060 Hrs ..... ** Designates Estimation(s) Using ASSUMED Value(s) ---------- SUMMARY (AOP v1.91): OZONE REACTION ---------- ****** NO OZONE REACTION ESTIMATION ****** (ONLY Olefins and Acetylenes are Estimated) Experimental Database: NO Structure Matches Fraction sorbed to airborne particulates (phi): 0.914 (Junge,Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation
Test substance	:	Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability	:	(2) valid with restrictions Acceptable method of estimation.
Flag	:	Critical study for SIDS endpoint

14.12.2007 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	

Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (2)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	

Method	:	The Fugacity was determined using the EQC Level III model as found in EPIWIN v3.20. An experimentally determined melting point value of 350 deg C for 2,5-dichlorophenol sodium salt was used. All other parameters used were the default values found in EPIWIN. Equal emissions to air, soil and water were used.
Result	:	Level III Fugacity Model (Full-Output): ========== Chem Name : Molecular Wt: 201.09 Henry's LC : 3e-014 atm-m3/mole (calc VP/Wsol) Vapor Press : 2.08e-011 mm Hg (Mpbpwin program) Liquid VP : 3.41e-008 mm Hg (super-cooled) Melting Pt : 350 deg C (user-entered)

Log Kow : 0.12 (Kowwin program)
Soil Koc : 0.54 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.14e-005	58.1	1000
Water	45.6	900	1000
Soil	54.3	1.8e+003	1000
Sediment	0.0886	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (%)	Advection (%)
Air	1.49e-17	0.00401	0.00336	0.000134	0.000112
Water	1e-18	1.04e+3	1.35e+3	34.5	44.9
Soil	4.25e-17	618	0	20.6	0
Sediment	9.62e-19	0.224	0.0523	0.00746	0.00174

Persistence Time: 984 hr
Reaction Time: 1.79e+003 hr
Advection Time: 2.19e+003 hr
Percent Reacted: 55.1
Percent Advected: 44.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 58.13
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.342 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : Phenol, 2,5-dichloro-, potassium salt, CAS Number 68938-81-8
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
14.12.2007 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Contact time : 4 day(s)
Degradation : = 54 - (±) % after 4 day(s)
Result :

Remark : The free phenol form of this material is reported to undergo 54% ring degradation in 4 days with acclimated sludge, it cannot be determined if this test substance is considered readily biodegradable by OECD criteria.
Result : The biological degradation of chlorophenols in activated sludge was

studied. 2,5-Dichlorophenol was more resistent to degradation than 2,4-dichlorophenol. While 2,4-dichlorophenol was 100% degraded, including ring degradation, in five days, 2,5-dichlorophenol was only 52% ring-degraded in four days. [USEPA; Ambient Water Quality Criteria Doc: Chlorinated Phenols p.C-29 (1980) EPA 440/5-80-032]**PEER REVIEWED** As cited in HSDB record for 2,5-dichlorophenol, update of 8-09-200

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichlorophenol CAS 583-79-8
Reliability : (2) valid with restrictions
Acceptable method of estimation.
Flag : Critical study for SIDS endpoint
14.12.2007 (3)

Deg. product :
Method : other: estimated
Year :
GLP : no
Test substance : other TS

Method : Estimation using BIOWIN v4.10 in EPIWIN v3.20. Experimentally determined melting point value of 350 deg C for 2,5-dichlorophenol sodium salt was used. All other parameters used were the default values found in EPIWIN.
Result : BIOWIN v4.10 predicts that dichlorophenol potassium salt is not readily biodegradable with primary biodegradation occurring in weeks and ultimate biodegradation occurring in weeks-months.

BIOWIN (v4.10) Program Results:
==========
SMILES : O(K)c1c(CL)ccc(CL)c1
CHEM :
MOL FOR: C6 H3 CL2 O1 K1
MOL WT : 201.09
---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Weeks
Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

Test substance : CAS 68938-81-8, 2,5-dichlorophenol potassium salt
Reliability : (2) valid with restrictions
Acceptable method of estimation.
14.12.2007 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

(1) EPI Suite, U.S. Environmental Protection Agency, 2000 - 2007.

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(3) Ingols RS et al; J Water Pollut Control Fed 38: 629-35 (1966) As cited in HSDB update of 8-09-2001

(4) EPI Suite v3.20, U.S. Environmental Protection Agency, 2000-2007.